This Page Is Inserted by IFW Operations
and is not a part of the Official Record

# BEST AVAILABLE IMAGES

Defective images within this document are accurate representations of
the original documents submitted by the applicant.

Defects in the images may include (but are not limited to):

- BLACK BORDERS

- TEXT CUT OFF AT TOP, BOTTOM OR SIDES

- FADED TEXT

- ILLEGIBLE TEXT

- SKEWED/SLANTED IMAGES

- COLORED PHOTOS

- BLACK OR VERY BLACK AND WHITE DARK PHOTOS

- GRAY SCALE DOCUMENTS

# IMAGES ARE BEST AVAILABLE COPY.

# As rescanning documents *will not* correct images, please do not report the images to the Image Problem Mailbox.

BMS-0010 AB

# PCT

## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(54) Title: CRYSTALLIZABLE COMPOSITIONS COMPRISING A HEPATITIS C VIRUS NS3 PROTEASE DOMAIN/NS4A COMPLEX AND CRYSTALS THEREBY OBTAINED

(57) Abstract

The present invention relates to compositions and crystals of a hepatitis C virus protease in complex with its viral cofactor. This invention also relates to methods of using the structure coordinates of hepatitis C virus protease in complex with a synthetic NS4A to solve the structure of similar or homologous proteins or protein complexes.

CRYSTALLIZABLE COMPOSITIONS COMPRISING A HEPATITIS C VIRUS NS3 PROTEASE DOMAIN/NS4A COMPLEX AND CRYSTALS THEREBY OBTAINED

5                     TECHNICAL FIELD OF INVENTION

The present invention relates to compositions and crystals of a hepatitis C virus protease in complex with its viral cofactor.  This invention also relates
10    to methods of using the structure coordinates of hepatitis C virus protease in complex with a synthetic NS4A to solve the structure of similar or homologous proteins or protein complexes.

15                     BACKGROUND OF THE INVENTION

Infection by hepatitis C virus (HCV) is a compelling human medical problem.  HCV is recognized as the causative agent for most cases of non-A, non-B
20    hepatitis, with an estimated human seroprevalence of 1% globally [Choo, Q.-L. et al., "Isolation of a cDNA Clone Derived From a Blood-Borne Non-A, Non-B Viral Hepatitis Genome", Science, 244, pp. 359-362 (1989); Kuo, G. et al., "An Assay for Circulating Antibodies to
25    a Major Etiologic Virus of Human Non-A, Non-B Hepatitis", Science, 244, pp. 362-364 (1989); Purcell, R.H., "Hepatitis C virus:  Historical perspective and current concepts", FEMS Microbiology Reviews, 14, pp. 181-192 (1994); Van der Poel, C.L., "Hepatitis C Virus.
30    Epidemiology, Transmission and Prevention in Hepatitis C virus.  Current Studies in Hematology and Blood Transfusion, H.W. Reesink, Ed., (Basel: Karger), pp. 137-163 (1994)].  Four million individuals may be

- 2 -

infected in the United States alone [Alter, M.J. and
Mast, E.E., "The Epidemiology of Viral Hepatitis in
the United States, Gastroenterol. Clin. North Am., 23,
pp. 437-455 (1994)].

5            Upon first exposure to HCV only about 20% of
infected individuals develop acute clinical hepatitis
while others appear to resolve the infection
spontaneously.  In most instances, however, the virus
establishes a chronic infection that persists for
10     decades [Iwarson, S. "The Natural Course of Chronic
Hepatitis", FEMS Microbiology Reviews, 14, pp. 201-204
(1994)].  This usually results in recurrent and
progressively worsening liver inflammation, which often
leads to more severe disease states such as cirrhosis
15     and hepatocellular carcinoma [Kew, M.C., "Hepatitis C
and Hepatocellular Carcinoma", FEMS Microbiology
Reviews, 14, pp. 211-220 (1994); Saito, I., et al.
"Hepatitis C Virus Infection is Associated with the
Development of Hepatocellular Carcinoma", Proc. Natl.
20     Acad. Sci. USA 87, pp. 6547-6549 (1990)].  Currently,
there are no broadly effective treatments for the
debilitating progression of chronic HCV.
           The HCV genome encodes a polyprotein of 3010-
3033 amino acids (Figure 1) [Choo, Q.-L., et al.
25     "Genetic Organization and Diversity of the Hepatitis C
Virus", Proc. Natl. Acad. Sci. USA, 88, pp. 2451-2455
(1991); Kato, N. et al., Molecular Cloning of the Human
Hepatitis C Virus Genome From Japanese Patients with
Non-A, Non-B Hepatitis", Proc. Natl. Acad. Sci. USA,
30     87, pp. 9524-9528 (1990); Takamizawa, A. et al.,
"Structure and Organization of the Hepatitis C Virus
Genome Isolated From Human Carriers", J. Virol., 65,
pp. 1105-1113 (1991)].  The HCV nonstructural (NS)

- 3 -

proteins provide catalytic machinery for viral
replication.  The NS proteins are derived by
proteolytic cleavage of the polyprotein
[Bartenschlager, R. et al., "Nonstructural Protein 3 of
5   the Hepatitis C Virus Encodes a Serine-Type Proteinase
Required for Cleavage at the NS3/4 and NS4/5
Junctions", J. Virol., 67, pp. 3835-3844 (1993);
Grakoui, A. et al. "Characterization of the Hepatitis C
Virus-Encoded Serine Proteinase:  Determination of
10  Proteinase-Dependent Polyprotein Cleavage Sites", J.
Virol., 67, pp. 2832-2843 (1993); Grakoui, A. et al.,
Expression and Identification of Hepatitis C Virus
Polyprotein Cleavage Products", J. Virol., 67, pp.
1385-1395 (1993); Tomei, L. et al., "NS3 is a serine
15  protease required for processing of hepatitis C virus
polyprotein", J. Virol., 67, pp. 4017-4026 (1993)].
        The HCV NS protein 3 (NS3) contains a serine
protease activity that helps process the majority of
the viral enzymes, and is thus considered essential for
20  viral replication and infectivity.  It is known that
mutations in the yellow fever virus NS3 protease
decreases viral infectivity [Chambers, T.J. et. al.,
"Evidence that the N-terminal Domain of Nonstructural
Protein NS3 From Yellow Fever Virus is a Serine
25  Protease Responsible for Site-Specific Cleavages in the
Viral Polyprotein", Proc. Natl. Acad. Sci. USA, 87, pp.
8898-8902 (1990)].  The first 181 amino acids of NS3
(residues 1027-1207 of the viral polyprotein) have been
shown to contain the serine protease domain of NS3 that
30  processes all four downstream sites of the HCV
polyprotein (Figure 1) [C. Lin et al., "Hepatitis C
Virus NS3 Serine Proteinase:  Trans-Cleavage

- 4 -

Requirements and Processing Kinetics", <u>J. Virol.</u>, 68, pp. 8147-8157 (1994)].

NS3 is associated with a cofactor, NS4A. NS4A seems critical to the activity of NS3, enhancing the proteolytic efficiency of NS3 at all of the cleavage sites. NS4A is a 54 residue amphipathic peptide, with a hydrophobic N-terminus and a hydrophilic C-terminus [Failla, C. et al., "Both NS3 and NS4A are Required for Proteolytic Processing of Hepatitis C Virus Nonstructural Proteins", <u>J. Virol.</u>, 68, pp. 3753-3760 (1994)]. Its function appears complex, possibly assisting in the membrane-localization of NS3 and other viral replicase components [Lin, C. et al. "A Central Region in the Hepatitis C Virus NS4A Protein Allows Formation of an Active NS3-NS4A Serine Proteinase Complex <u>In Vivo</u> and <u>In Vitro</u>", <u>J. Virol.</u>, 69, pp. 4373-4380 (1995b); Shimizu, Y. et al., "Identification of the Sequence on NS4A Required for Enhanced Cleavage of the NS5A/5B Site by Hepatitis C Virus NS3 Protease", <u>J. Virol.</u>, 70, pp. 127-132 (1996); Tanji, Y. et al., "Hepatitis C Virus-Encoded Nonstructural Protein NS4A has Versatile Functions in Viral Protein Processing", <u>J. Virol.</u>, 69, pp. 1575-1581 (1995)] but its best characterized function is that of a cofactor for the NS3 protease.

The current understanding of HCV has not led to satisfactory treatments for HCV infection. The prospects for effective anti-HCV vaccines remain uncertain. The only established therapy for HCV disease is interferon treatment. However, interferons have significant side effects [Janssen, H. L. A., et al. "Suicide Associated with Alfa-Interferon Therapy for Chronic Viral Hepatitis", <u>J. Hepatol.</u>, 21, pp. 241-

- 5 -

243 (1994)]; Renault, P.F. and Hoofnagle, J.H., "Side
effects of alpha interferon. Seminars in Liver Disease
9, 273-277. (1989)] and induce long term remission in
only a fraction (~ 25%) of cases [Weiland, O.
5      "Interferon Therapy in Chronic Hepatitis C Virus
Infection", FEMS Microbiol. Rev., 14, pp. 279-288
(1994)].  Thus, there is a need for more effective
anti-HCV therapies.

       The NS3 protease is considered a potential
10     target for antiviral agents.  However, drug discovery
efforts directed towards the NS3 protein have been
hampered by the lack of structural information about
NS3 and its complex with NS4A.  Such structural
information would provide valuable information in
15     discovery of HCV NS3 protease inhibitors.  However,
efforts to determine the structure of HCV NS3 protease
have been hampered by difficulties in obtaining
sufficient quantities of pure active enzyme
[Steinkuhler, C. et al., "In Vitro Activity of
20     Hepatitis C Virus Protease NS3 Purified from
Recombinant Baculovirus-Infected Sf9 Cells", J. Biol
Chem., pp. 637-6273 (1996)].  There have been no
crystals reported of any NS3 or NS3 protease domain
protein.  Thus, x-ray crystallographic analysis of such
25     proteins has not been possible.


                  SUMMARY OF THE INVENTION


       Applicants have solved this problem by
30     providing, for the first time, compositions comprising
a hepatitis C virus (HCV) NS3 protease-like polypeptide
complexed with a NS4A-like peptide and methods for
making such compositions.

- 6 -

The invention also provides crystals of a HCV
NS3 protease-like polypeptide/NS4A-like peptide complex
and methods for making such crystals.

The invention also provides the structure
5    coordinates of a HCV NS3 protease-like
polypeptide/NS4A-like peptide complex.

The invention also provides a method for
determining at least a portion of the three-dimensional
structure of molecules or molecular complexes which
10   contain at least some structurally similar features to
a HCV NS3 serine protease domain.


## BRIEF DESCRIPTION OF THE FIGURES


15        Figure 1 depicts HCV polyprotein processing.
The locations of the HCV structural and nonstructural
proteins are marked on a diagram of the 3011 amino acid
polypeptide.  Cleavages between the structural proteins
by cellular signal peptidases are marked by asterisks.
20   Cleavage between NS2 and NS3 is mediated by the NS2/NS3
metallo-protease.  The NS3 serine protease is
responsible for cleavages between NS3 and NS4A, NS4A
and NS4B, NS4B and NS5A, and NS5A and NS5B.

Figure 2 depicts stereo ribbon diagrams of
25   the NS3/NS4A complex.  The view is into the active site
cleft of the enzyme.  Side-chains of active site
residues His-1083, Asp-1107, and Ser-1165, along with
$Zn^{++}$ ligands Cys-1123, Cys-1125, and Cys-1171 are
displayed in ball-and-stick representation.  $Zn^{++}$, its
30   $H_2O$ ligand, and the β-strand formed by NS4A are also
shown.

- 7 -

Figure 3 lists the atomic structure coordinates for hepatitis C virus recombinant, truncated nonstructural protein 3 (hereafter referred to as tNS3) in complex with a synthetic peptide of the central region of the nonstructural protein 4A (hereafter referred to as sNS4A) as derived by X-ray diffraction from crystals of that complex (hereafter referred to as tNS3/sNS4A). The preparation of the complex is described in Examples 1 and 2. The following abbreviations are used in Figure 3:

"Atom type" refers to the element whose coordinates have been determined. Elements are defined by the first letter in the column except for zinc which is defined by the letters "Zn".

"X, Y, Z" crystallographically define the atomic position determined for each atom.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

Figure 4 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figures 5 and 6.

Figure 5 shows a cross section of a magnetic storage medium.

Figure 6 shows a cross section of a optically-readable data storage medium.

- 8 -

## DETAILED DESCRIPTION OF THE INVENTION

The following abbreviations are used throughout the application:

| | | |
|---|---|---|
| A = Ala = Alanine | | T = Thr = Threonine |
| V = Val = Valine | | C = Cys = Cysteine |
| L = Leu = Leucine | | Y = Tyr = Tyrosine |
| I = Ile = Isoleucine | | N = Asn = Asparagine |
| P = Pro = Proline | | Q = Gln = Glutamine |
| F = Phe = Phenylalanine | | D = Asp = Aspartic Acid |
| W = Trp = Tryptophan | | E = Glu = Glutamic Acid |
| M = Met = Methionine | | K = Lys = Lysine |
| G = Gly = Glycine | | R = Arg = Arginine |
| S = Ser = Serine | | H = His = Histidine |

HCV = hepatitis C virus

Additional definitions are set forth in the specification where necessary.

In order that the invention described herein may be more fully understood, the following detailed description is set forth.

Applicants have solved the above problems by providing, for the first time, crystallizable compositions comprising a HCV NS3 protease-like polypeptide in complex with a NS4A-like peptide.

Thus, in one embodiment of this invention is provided a composition comprising a hepatitis C virus NS3-like polypeptide in complex with an NS4A-like peptide.

The HCV NS3-like polypeptide portion of the complex is any polypeptide which has the serine protease activity of the naturally occurring HCV NS3A protease, particularly the ability to cleave the HCV

- 9 -

polyprotein.  It includes HCV NS3, NS3 protease domain
polypeptides and NS3 protease domain-like polypeptides.

As used herein, the terms "HCV NS3" and "NS3"
refers to the hepatitis C virus nonstructural-3 protein
5    as defined in Lin, C. et al., "Hepatitis C Virus NS3
Serine Proteinase:  *Trans*-Cleavage Requirements and
Processing Kinetics", J. Virol., 68, pp. 8147-8157
(1994).

The term "NS3 protease domain polypeptide"
10   refers to a truncated, serine protease portion of NS3
as defined in [Bartenschlager, R. et al.,
"Nonstructural Protein 3 of the Hepatitis C Virus
Encodes a Serine-Type Proteinase Required for Cleavage
at the NS3/4 and NS4/5 Junctions", J. Virol., 67, pp.
15   3835-3844 (1993); Grakoui, A. et al. "Characterization
of the Hepatitis C Virus-Encoded Serine Proteinase:
Determination of Proteinase-Dependent Polyprotein
Cleavage Sites", J. Virol., 67, pp. 2832-2843 (1993);
Grakoui, A. et al., Expression and Identification of
20   Hepatitis C Virus Polyprotein Cleavage Products", J.
Virol., 67, pp. 1385-1395 (1993); Tomei, L. et al.,
"NS3 is a serine protease required for processing of
hepatitis C virus polyprotein", J. Virol., 67, pp.
4017-4026 (1993)].  The disclosure of each of these
25   documents is herein incorporated by reference.

The term "NS3 protease domain-like
polypeptides" refers to polypeptides that differ from
NS3 protease domain polypeptides by having amino acid
deletions, substitutions, and additions, but which
30   retain the serine protease activity of NS3.

Preferably, the NS3-like polypeptide in the
compositions of this invention is tNS3, a recombinantly

- 10 -

produced hepatitis C virus protease domain protein that
is prepared as described herein.

  The NS4A-like peptide portion of the
compositions of this invention is any peptide or
5  peptide mimetic that is capable of acting as a NS4A
cofactor for the NS3.  These include NS4A, peptide
fragments thereof and other peptides that differ from
NS4A by having amino acid deletions, substitutions, and
additions, while retaining the above-described
10  activity.

  As used herein the term "NS4A" refers to the
hepatitis C virus nonstructural protein 4A which acts
as a cofactor for NS3 protease [Failla, C. et al.,
"Both NS3 and NS4A are Required for Proteolytic
15  Processing of Hepatitis C Virus Nonstructural Proteins"
J. Virol. 68, pp. 3753-3760 (1994); Lin, C. et al.,
"Hepatitis C Virus NS3 Serine Proteinase: Trans-
Cleavage Requirements and Processing Kinetics" J.
Virol. 68, pp. 8147-8157 (1994b)]

20  Preferably, the NS4A-like peptide is sNS4A,
the synthetic peptide H-KKGSVVIVGRIVLSGKPAIIPKK-OH.
This peptide encompasses the essential NS3 protease
domain residues of NS4A.

  Both the NS3-like polypeptide and the NS4A-
25  like peptide may be produced by any well-known method,
including synthetic methods, such as solid phase,
liquid phase and combination solid phase/liquid phase
syntheses; recombinant DNA methods, including cDNA
cloning, optionally combined with site directed
30  mutagenesis; and/or purification of the natural
products, optionally combined with enzymatic cleavage
methods to produce fragments of naturally occurring NS3
and NS4A.

- 11 -

According to a preferred embodiment, the
compositions of this invention are crystallizable.  In
this preferred embodiment all of the preferred choices
for the NS3-like polypeptide and the NS4A-like peptide
5    are identical to those indicated above.

Advantageously, the crystallizable
composition provided by this invention are amenable to
x-ray crystallography.  Thus, this invention also
provides the three-dimensional structure of an HCV NS3-
10   like polypeptide/NS4A-like peptide complex,
specifically an HCV tNS3/sNS4A complex, at 2.5 Å
resolution.  Importantly, this has provided for the
first time, information about the shape and structure
of the NS3 protease domain.

15   The three-dimensional structure of the HCV
tNS3/sNS4A complex of this invention is defined by a
set of structure coordinates as set forth in Figure 3.
The term "structure coordinates" refers to Cartesian
coordinates derived from mathematical equations related
20   to the patterns obtained on diffraction of a
monochromatic beam of X-rays by the atoms (scattering
centers) of an tNS3/sNS4A complex in crystal form.  The
diffraction data are used to calculate an electron
density map of the repeating unit of the crystal.  The
25   electron density maps are then used to establish the
positions of the individual atoms of the tNS3/sNS4A
enzyme or enzyme complex.

Those of skill in the art will understand
that a set of structure coordinates for an enzyme or an
30   enzyme-complex or a portion thereof, is a relative set
of points that define a shape in three dimensions.
Thus, it is possible that an entirely different set of
coordinates could define a similar or identical shape.

- 12 -

Moreover, slight variations in the individual coordinates will have little effect on overall shape.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth in Figure 3 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same.

Various computational analyses are therefore necessary to determine whether a molecule or molecular complex or a portion thereof is sufficiently similar to all or parts of the NS3-like polypeptide/NS4A-like peptide structure described above as to be considered the same. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different

- 13 -

conformations of the same structure, and different
parts of the same structure.  The procedure used in
Molecular Similarity to compare structures is divided
into four steps:  1) load the structures to be
5     compared; 2) define the atom equivalences in these
structures; 3) perform a fitting operation; and 4)
analyze the results.

Each structure is identified by a name.  One
structure is identified as the target (i.e., the fixed
10    structure); all remaining structures are working
structures (i.e., moving structures).  Since atom
equivalency within QUANTA is defined by user input, for
the purpose of this invention we will define equivalent
atoms as protein backbone atoms (N, $C\alpha$, C and O) for
15    all conserved residues between the two structures being
compared.  We will also consider only rigid fitting
operations.

When a rigid fitting method is used, the
working structure is translated and rotated to obtain
20    an optimum fit with the target structure.  The fitting
operation uses an algorithm that computes the optimum
translation and rotation to be applied to the moving
structure, such that the root mean square difference of
the fit over the specified pairs of equivalent atom is
25    an absolute minimum.  This number, given in angstroms,
is reported by QUANTA.

For the purpose of this invention, any
molecule or molecular complex that has a root mean
square deviation of conserved residue backbone atoms
30    (N, $C\alpha$, C, O) of less than 1.5 Å when superimposed on
the relevant backbone atoms described by structure
coordinates listed in Figure 3 are considered

- 14 -

identical. More preferably, the root mean square
deviation is less than 1.0 Å.

The term "root mean square deviation" means
the square root of the arithmetic mean of the squares
5    of the deviations from the mean. It is a way to
express the deviation or variation from a trend or
object. For purposes of this invention, the "root mean
square deviation" defines the variation in the backbone
of a protein or protein complex from the relevant
10   portion of the backbone of the NS3-like polypeptide
portion of the complex as defined by the structure
coordinates described herein.

Once the structure coordinates of a protein
crystal have been determined they are useful in solving
15   the structures of other crystals.

Thus, in accordance with the present
invention, the structure coordinates of a NS3-like
polypeptide/NS4A-like peptide complex, and in
particular a tNS3/sNS4A complex, and portions thereof
20   is stored in a machine-readable storage medium. Such
data may be used for a variety of purposes, such as
drug discovery and x-ray crystallographic analysis or
protein crystal.

Accordingly, in one embodiment of this
25   invention is provided a machine-readable data storage
medium comprising a data storage material encoded with
the structure coordinates set forth in Figure 3.

Figure 4 demonstrates one version of these
embodiments. System 10 includes a computer 11
30   comprising a central processing unit ("CPU") 20, a
working memory 22 which may be, e.g, RAM (random-access
memory) or "core" memory, mass storage memory 24 (such
as one or more disk drives or CD-ROM drives), one or

- 15 -

more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bidirectional system bus 50.

Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 36 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

In operation, CPU 20 coordinates the use of the various input and output devices 36, 46, coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to

- 16 -

components of the hardware system 10 are included as
appropriate throughout the following description of the
data storage medium.

   Figure 5 shows a cross section of a magnetic
5 data storage medium 100 which can be encoded with a
machine-readable data that can be carried out by a
system such as system 10 of Figure 4.  Medium 100 can
be a conventional floppy diskette or hard disk, having
a suitable substrate 101, which may be conventional,
10 and a suitable coating 102, which may be conventional,
on one or both sides, containing magnetic domains (not
visible) whose polarity or orientation can be altered
magnetically.  Medium 100 may also have an opening (not
shown) for receiving the spindle of a disk drive or
15 other data storage device 24.

   The magnetic domains of coating 102 of medium
100 are polarized or oriented so as to encode in manner
which may be conventional, machine readable data such
as that described herein, for execution by a system
20 such as system 10 of Figure 4.

   Figure 6 shows a cross section of an
optically-readable data storage medium 110 which also
can be encoded with such a machine-readable data, or
set of instructions, which can be carried out by a
25 system such as system 10 of Figure 4.  Medium 110 can
be a conventional compact disk read only memory
(CD-ROM) or a rewritable medium such as a
magneto-optical disk which is optically readable and
magneto-optically writable.  Medium 100 preferably has
30 a suitable substrate 111, which may be conventional,
and a suitable coating 112, which may be conventional,
usually of one side of substrate 111.

- 17 -

In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which preferably is substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

For the first time, the present invention permits the use of structure-based or rational drug design techniques to design, select, and synthesize chemical entities, including inhibitory compounds that are capable of binding to HCV NS3, NS4A, NS3/NS4A complex, or any portion thereof.

One particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a compound by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes.

Those of skill in the art will realize that association of natural ligands or substrates with the binding pockets of their corresponding receptors or

- 18 -

enzymes is the basis of many biological mechanisms of action. The term "binding pocket", as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates

5   with another chemical entity or compound. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or any parts of the binding pockets. An understanding of such

10  associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential ligands or inhibitors of receptors

15  or enzymes, such as inhibitors of HCV NS3-like polypeptides, and more importantly HCV NS3.

The term "associating with" refers to a condition of proximity between chemical entities or compounds, or portions thereof. The association may be

20  non-covalent -- wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions -- or it may be covalent.

In iterative drug design, crystals of a

25  series of protein/compound complexes are obtained and then the three-dimensional structures of each complex is solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds

30  with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex

- 19 -

and previously solved protein/compound complexes.  By
observing how changes in the compound affected the
protein/compound associations, these associations may
be optimized.

5          In some cases, iterative drug design is
carried out by forming successive protein-compound
complexes and then crystallizing each new complex.
Alternatively, a pre-formed protein crystal is soaked
in the presence of an inhibitor, thereby forming a
10    protein/compound complex and obviating the need to
crystallize each individual protein/compound complex.
Advantageously, the HCV NS3-like polypeptide/NS4A-like
peptide crystals, and in particular the tNS3/sNS4A
crystals, provided by this invention may be soaked in
15    the presence of a compound or compounds, such as NS3
protease inhibitors, to provide NS3-like
polypeptide/NS4A-like peptide /compound crystal
complexes.

          As used herein, the term "soaked" refers to a
20    process in which the crystal is transferred to a
solution containing the compound of interest.

          In another embodiment of this invention is
provided a method for preparing a composition
comprising a NS3-like polypeptide protein comprising
25    the steps described in Examples 1 and 2.  Preferably,
the composition comprises a NS3-like polypeptide in
complex with a NS4A-like peptide.

          The structure coordinates set forth in Figure
3 can also be used to aid in obtaining structural
30    information about another crystallized molecule or
molecular complex.  This may be achieved by any of a
number of well-known techniques, including molecular
replacement.

- 20 -

The structure coordinates set forth in Figure
3 can also be used for determining at least a portion
of the three-dimensional structure of molecules or
molecular complexes which contain at least some
structurally similar features to HCV NS3.  In
particular, structural information about another
crystallized molecule or molecular complex may be
obtained.  This may be achieved by any of a number of
well-known techniques, including molecular replacement.

Therefore, in another embodiment this
invention provides a method of utilizing molecular
replacement to obtain structural information about a
crystallized molecule or molecular complex whose
structure is unknown comprising the steps of:

a) generating an X-ray diffraction pattern
from said crystallized molecule or molecular complex;
and

b) applying at least a portion of the
structure coordinates set forth in Figure 3 to the
X-ray diffraction pattern to generate a
three-dimensional electron density map of the molecule
or molecular complex whose structure is unknown.

Preferably, the crystallized molecule or
molecular complex comprises a NS3-like polypeptide and
a NS4A-like peptide.  More preferably, the crystallized
molecule or molecular complex is obtained by soaking a
crystal of this invention in a solution.

By using molecular replacement, all or part
of the structure coordinates of the tNS3/sNS4A complex
provided by this invention (and set forth in Figure 3)
can be used to determine the structure of a
crystallized molecule or molecular complex whose
structure is unknown more quickly and efficiently than
attempting to determine such information ab initio.

- 21 -

        Molecular replacement provides an accurate
estimation of the phases for an unknown structure.
Phases are a factor in equations used to solve crystal
structures that can not be determined directly.
5       Obtaining accurate values for the phases, by methods
other than molecular replacement, is a time-consuming
process that involves iterative cycles of
approximations and refinements and greatly hinders the
solution of crystal structures.  However, when the
10      crystal structure of a protein containing at least a
homologous portion has been solved, the phases from the
known structure provide a satisfactory estimate of the
phases for the unknown structure.
        Thus, this method involves generating a
15      preliminary model of a molecule or molecular complex
whose structure coordinates are unknown, by orienting
and positioning the relevant portion of the tNS3/sNS4A
complex according to Figure 3 within the unit cell of
the crystal of the unknown molecule or molecular
20      complex so as best to account for the observed X-ray
diffraction pattern of the crystal of the molecule or
molecular complex whose structure is unknown.  Phases
can then be calculated from this model and combined
with the observed X-ray diffraction pattern amplitudes
25      to generate an electron density map of the structure
whose coordinates are unknown.  This, in turn, can be
subjected to any well-known model building and
structure refinement techniques to provide a final,
accurate structure of the unknown crystallized molecule
30      or molecular complex [E. Lattman, "Use of the Rotation
and Translation Functions", in Meth. Enzymol., 115, pp.
55-77 (1985); M. G. Rossmann, ed., "The Molecular
Replacement Method", Int. Sci. Rev. Ser., No. 13,
Gordon & Breach, New York (1972)].

- 22 -

The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the tNS3/sNS4A complex can be solved by this method.

In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about a molecule or molecular complex, wherein the complex comprises a NS3-like polypeptide. Preferably the NS3-like polypeptide is tNS3 or homologue thereof.

The structure coordinates of tNS3/sNS4A as provided by this invention are particularly useful in solving the structure of other crystal forms of NS3-like polypeptide, preferably other crystal forms of tNS3; NS3-like polypeptide/NS4A-like peptide, preferably tNS3/sNS4A; or complexes comprising any of the above.

The structure coordinates are also particularly useful to solve the structure of crystals of NS3-like polypeptide/NS4A-like peptide complexes, particularly tNS3/sNS4A, co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including interaction of candidate NS3 inhibitors with NS3 or the NS3/NS4A complex. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their NS3 inhibition activity.

- 23 -

All of the complexes referred to above may be
studied using well-known X-ray diffraction techniques
and may be refined versus 1.5-3 Å resolution X-ray data
to an R value of about 0.20 or less using computer
5  software, such as X-PLOR [Yale University, ©1992,
distributed by Molecular Simulations, Inc.; see, e.g.,
Blundell & Johnson, supra; Meth. Enzymol., vol. 114 &
115, H. W. Wyckoff et al., eds., Academic Press
(1985)]. This information may thus be used to optimize
10 known NS3 inhibitors, and more importantly, to design
new NS3 inhibitors.

In order that this invention be more fully
understood, the following examples are set forth.
These examples are for the illustrative purposes only
15 and are not to be construed as limiting the scope of
this invention in any way.


EXAMPLE 1
Expression and Purification of tNS3
20     The truncated NS3 serine protease domain
(tNS3) was cloned from a cDNA of the hepatitis C virus
H strain [Grakoui, A. et al., "Expression and
Identification of Hepatitis C Virus Polyprotein
Cleavage Products", J. Virol., 67, pp. 1385-1395
25 (1993)]. The first 181 amino acids of NS3 (residues
1027-1207 of the viral polyprotein) have been shown to
contain the serine protease domain of NS3 that
processes all four downstream sites of the HCV
polyprotein [Lin, C., et al., Hepatitis C Virus NS3
30 Serine Proteinase: Trans-Cleavage Requirements and
Processing Kinetics", J. Virol. 68, pp. 8147-8157
(1994b)], so we expressed a (His)$_6$-fusion protein based
on this tNS3. The plasmid pET-BS(+)/HCV/T7-NS3$_{181}$-His

- 24 -

was derived from pTM3/HCV/1027-1207 (NS3$_{181}$) (Id.), by using polymerase chain reaction to introduce epitope tags and new restriction sites. A T7-tag (ASMTGGQQMG), from the N-terminus of the gene 10 protein of the T7 bacteriophage

[Tsai, D.E. et al., "*In Vitro* Selection of an RNA Epitope Immunologically Cross-Reactive With a Peptide", Proc. Natl. Acad. Sci. USA, 89, pp. 8864-8868 (1992)], was placed at the N-terminus of the tNS3 domain. Two linker residues (GS) were placed at the tNS3 C-terminus, followed by the (His)$_6$-tag. *E.coli* JM109(DE3) cells, freshly transformed with the pET-BS(+)/HCV/T7-NS3$_{181}$-His plasmid, were grown at 37 °C in complex media supplement with 100 µg/ml ampicillin, in a 10 L fermentor (Braun). When the cell density reached an OD$_{600}$ of 3-4 the temperature of the culture was rapidly reduced to 30 °C, and induction was immediately initiated by the addition of 1 mM IPTG. Cells were harvested at 2 h post-induction, and flash frozen at -70 °C prior to purification.

The tNS3 was purified from the soluble fraction of the recombinant *E.coli* lysates as follows, with all procedures being performed at 4 °C unless stated otherwise. Cell paste (75-100g) was resuspended in 15 volumes of 50 mM HEPES, 0.3 M NaCl, 10% glycerol, 0.1% ß-octyl glucoside, 2 mM ß-mercaptoethanol, pH 8.0. Cells were ruptured using a microfluidizer and the homogenate was clarified by centrifugation at 100,000 x g for 30 min. The supernatant was brought to 50 mM HEPES, 20 mM imidazole, 0.3 M NaCl, 27.5% glycerol, 0.1% ß-octyl- glucoside, 2 mM ß-mercaptoethanol, pH 8.0, and applied at 1.0 ml/min to a 7.0 ml Ni-Agarose

- 25 -

affinity column, equilibrated in the same buffer.
After loading, the column was washed with 10-15 volumes
of equilibration buffer and the bound proteins were
eluted with equilibration buffer containing 0.35 M
5      imidazole.  The protein was then size-fractionated on
two columns in series (each 2.6 cm x 90 cm) packed with
Pharmacia high resolution S100 resin and equilibrated
with 25 mM HEPES, 0.3M NaCl, 10% glycerol, 0.1% ß-
octylglucoside, 2 mM ß-mercaptoethanol, pH 8.0.  The
10     tNS3 fractions, identified by SDS-PAGE, were pooled and
concentrated to 1 mg/ml using a Amicon Centriprep-10,
and stored at -70°C.  The tNS3 was thawed slowly on ice
and the NS4A peptide (dissolved in the size-exclusion
chromatography buffer) was added at a tNS3:NS4A-peptide
15     molar ratio of 1:2.  The sample was then diluted 2.5-
fold with 15 mM MES, 0.5 M NaCl, 20 mM ß-
mercaptoethanol, pH6.5, and concentrated to ~2 ml (~ 2
mg/ml) by ultrafiltration.  The sample was then diluted
2-fold with the pH 6.5 buffer and concentrated again to
20     ~2 ml.  This dilution process was repeated until it
gave a >40-fold dilution of the original buffer
constituents.  The protein sample was then concentrated
to 13.0 mg/ml and centrifuged at ~300,000 x g for 20
min at 4 °C.  Concentrations of the pure tNS3 and
25     tNS3/4A complex were determined by UV absorption
spectroscopy, using a molar absorption coefficient
$(A_{280})$ of 17,700 $M^{-1}.cm^{-1}$.


## EXAMPLE 2

### 4A Peptide Synthesis and Purification

30          The HCV NS4A peptide was synthesized to span
residues Gly21 to Pro39 of the viral cofactor (residues

- 26 -

1678 to 1696 of the HCV polyprotein), which
incorporates the essential region reported to be
essential for NS3 stimulation [Lin, C. et al. "A
Central Region in the Hepatitis C Virus NS4A Protein
Allows Formation of an Active NS3-NS4A Serine
Proteinase Complex In Vivo and In Vitro", J. Virol. 69,
pp. 4373-4380 (1995)].  Lysine residues were added to
the termini to assist aqueous solubility, and a serine
residue was substituted for Cys22 (residue 1679 of the
polyprotein of the HCV H strain).  The peptide (H-
KKGSVVIVGRIVLSGKPAIIPKK-OH · TFA salt) was prepared by
the solid-phase peptide synthesis (Applied Biosystems
433A) beginning with $N^a$-Fmoc, $N^e$-Boc-Lys Wang resin.
$N^a$-Fmoc-protected amino acids were added sequentially
using HBTU (2-(1H-benzotriazol-1-yl)1,1,3,3-
tetramethyluronium hexafluorophosphate) with HOBt (1-
hydroxybenzotriazole hydrate) as coupling agents in N-
methylpyrrolidinone.  Cleavage from the resin and
global deprotection were accomplished with 95%
trifluoroacetic acid and 5% water at room temperature
for 1.5 hr (15 ml/ g resin).  The peptide was purified
by preparative HPLC on a Waters Delta Pak C18, 15 μm,
300Å column (30 mm x 300 mm) eluting with a linear
gradient of acetonitrile (15-40%) in 0.1% aqueous
trifluoroacetic acid over 35 min (flow rate of 22
ml/min).  Peptide purity was confirmed by analytical
HPLC.  The sequence was confirmed by direct N-terminal
sequence analysis and matrix-assisted laser desorption
mass spectrometry (Kratos MALDI I), which showed the
correct $(M + H)^+$ and $(M + Na)^+$ molecular ions.

- 27 -

## EXAMPLE 3
### Crystallization and Data Collection

Crystals of the tNS3/NS4A complex were grown
by hanging-drop vapor diffusion over a reservoir of 0.1
M MES, 1.8 M NaCl, 0.1 M sodium/potassium phosphate, 10
mM ß-mercaptoethanol, pH 6.5. The crystals grew over
the course of 2-3 weeks, to final dimensions of about
0.1 x 0.1 x 0.25 mm. The rhombohedral crystals used in
this study belonged to space group R32, with unit cell
dimensions a=b=225.0Å, and c=75.5Å, and contained two
tNS3/NS4A complexes per asymmetric unit.

Statistics for data collection, heavy atom
refinement, and crystallographic refinement are given
in Table 1. All heavy atom soaks were done in hanging-
drops over the same reservoir as used for
crystallization. Crystals were transferred to a
stabilizing solution (50 mM MES, 2.0 M NaCl, 0.1 M
sodium/potassium phosphate, 10 mM ß-mercaptoethanol,
and 20% glycerol, pH 6.2) and then frozen in a dry
nitrogen gas stream at 100 K (Molecular Structure
Corp., Houston, TX) for data collection. Data was
acquired by oscillation photography on a Rigaku R-AXIS
IIC phosphor imaging area detector mounted on a Rigaku
RU200 rotating anode generator (MSC), operating at 50kV
and 100mA. Measured intensities were integrated,
scaled, and merged using the HKL software package (Z.
Otwinowski and W. Minor).

## EXAMPLE 4
### Phasing, Model Building and Refinement

Heavy atom positions were located by
inspection and confirmed with difference Fourier
syntheses. Heavy atom parameters were refined and

- 28 -

phases computed to 3.1Å using the program PHASES
[Furey, W. and Swaminathan, S. "PHASES-95: a program
package for the processing and analysis of diffraction
data from macromolecules", Meth. Enzymol., (1996). MIR
phases were improved and extended to 2.7Å by cycles of
solvent flattening [Wang, B.C., "Resolution of Phase
Ambiguity in Macromolecular Crystallography", Methods
in Enzymol. 115, pp. 90-112 (1985)] combined with
histogram matching [Zhang, K.Y.J. and Main, P., "The
Use of Sayre's Equation With Solvent Flattening and
Histogram Matching for Phase Extension and Refinement
of Protein Structures", Acta Crystallogr., A46, pp.
377-381 (1990)] using the CCP4 crystallographic package
(Collaborative Computation Project, 1994). The
resulting electron density map displayed nearly
continuous density for the protein backbone as well as
strong side chain density. Approximately 80% of the
model could be unambiguously built into this map
(QUANTA 4.1, Molecular Simulations), and a single round
of simulated annealing refinement in X-PLOR [Brunger,
A. T., "X-PLOR: A System for X-Ray Crystallography and
NMR", New Haven, Connecticut: Department of Molecular
Biophysics and Biochemistry, Yale University (1993)]
brought the R-factor to 29% and free R value to 33%
[Brunger, A. T., "Free R Value: A Novel Statistical
Quantity for Assessing the Accuracy of Crystal
Structures", Nature, 355, pp. 472-475 (1992)]. The
remainder of the model was built and refined in several
steps, by first extending the resolution to 2.5Å and
then adding well-ordered water molecules. A final
round of positional and individual temperature factor
refinement brought the R-factor to 21.6% (free R value
26.1%) for 26,652 reflections between 6.0 and 2.5Å

- 29 -

(F>1sF). The current model consisted of tNS3 residues 1055-1206 and NS4A residues 1678-1693 in complex A, and tNS3 residues 1028-1206 and NS4A residues 1678-1696 for complex B (polyprotein numbering, with 2 zinc atoms and 130 water molecules. A Ramachandran plot for the final model contained 91% of the residues in the most favored regions and 0% in disallowed or generously-allowed regions. The rms deviations from ideality were 0.007Å for bond lengths and 1.47° for bond angles.

While we have described a number of embodiments of this invention, it is apparent that our basic examples may be altered to provide other embodiments which utilize the products and processes of this invention. Therefore, it will be appreciated that the scope of this invention is to be defined by the appended claims rather than by the specific embodiments which have been represented by way of example.

- 30 -

## CLAIMS

We claim:

1.    A composition comprising a HCV NS3-like polypeptide complexed with a NS4A-like peptide.

2.    The composition according to claim 1, wherein the HCV NS3-like polypeptide is a NS3 protease domain polypeptide or a NS3 protease domain-like polypeptide.

3.    The composition according to claim 1, wherein the HCV NS3-like polypeptide is tNS3.

4.    The composition according to any one of claims 1 to 3, wherein the NS4A-like peptide is H-KKGSVVIVGRIVLSGKPAIIPKK-OH.

5.    A crystal comprising a HCV NS3-like polypeptide complexed with a NS4A-like peptide.

6.    The crystal according to claim 5, wherein the HCV NS3-like polypeptide is a NS3 protease domain polypeptide or a NS3 protease domain-like polypeptide.

7.    The crystal according to claim 5, wherein the HCV NS3-like polypeptide is tNS3.

8.    The crystal according to any one of claims 1 to 3, wherein the NS4A-like peptide is H-KKGSVVIVGRIVLSGKPAIIPKK-OH.

- 31 -

9.  The crystal according to claim 5,
additionally comprising an inhibitor of HVC NS3.

10.  A machine-readable data storage medium,
comprising a data storage material encoded with machine
readable data, wherein the data is defined by the
structure coordinates of a tNS3/sNS4A complex according
to Figure 3, or a homologue of said complex, wherein
said homologue comprises backbone atoms that have a
root mean square deviation from the backbone atoms of
the complex of not more than 1.5A

11.  The machine-readable data storage
medium, according to claim 10, wherein said molecule or
molecular complex is defined by the set of structure
coordinates for tNS3/sNS4A according to Figure 3, or a
homologue of said molecule or molecular complex, said
homologue having a root mean square deviation from the
backbone atoms of said amino acids of not more than 1.5
Å.

12.  A machine-readable data storage medium
comprising a data storage material encoded with a first
set of machine readable data comprising a Fourier
transform of at least a portion of the structural
coordinates for tNS3/sNS4A according to Figure 3;
which, when combined with a second set of machine
readable data comprising an X-ray diffraction pattern
of a molecule or molecular complex of unknown
structure, using a machine programmed with instructions
for using said first set of data and said second set of
data, can determine at least a portion of the structure
coordinates corresponding to the second set of machine

- 32 -

readable data, said first set of data and said second set of data.

5      13.   A method of obtaining structural information about a molecule or a molecular complex of unknown structure by using the structure coordinates set forth in Figure 3, comprising the steps of:
       a.    generating X-ray diffraction data from said crystallized molecule or molecular complex;
10            b.    applying at least a portion of the structure coordinates set forth in Figure 3 to said X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.
15

       14.   The method according to claim 13, wherein the molecule or molecular complex of unknown structure comprises a polypeptide selected from a NS3-like polypeptide in complex with a NS4A-like peptide.

## Fig. 1
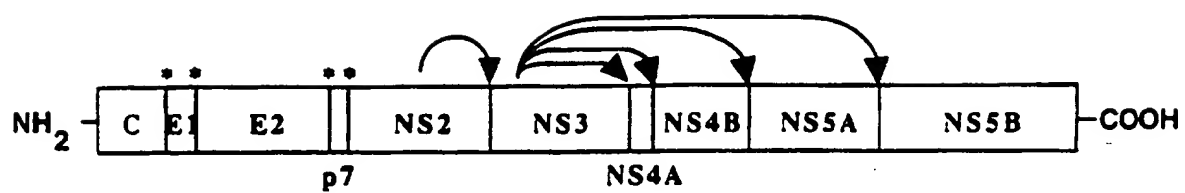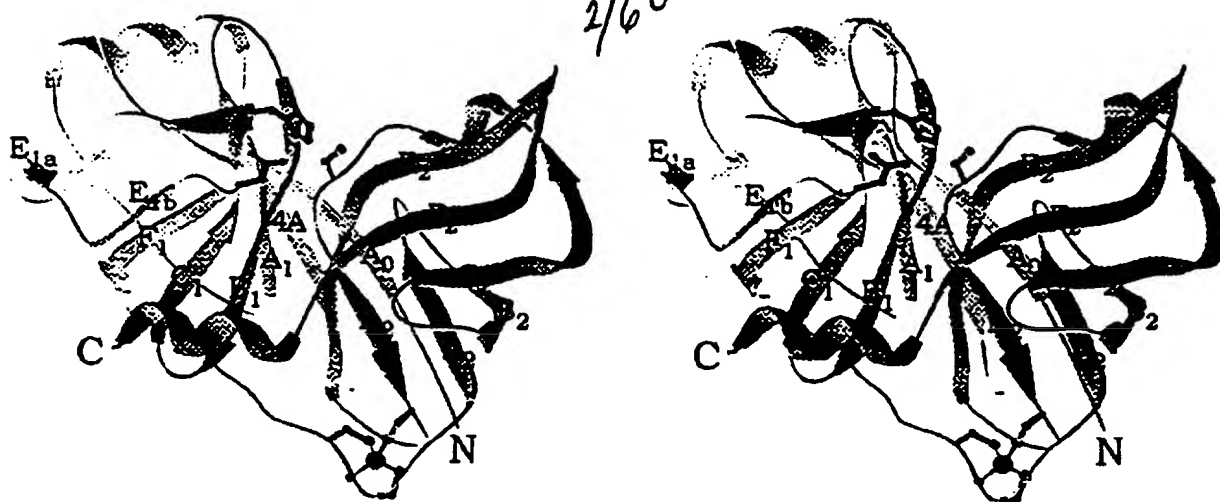
Figure 2

## FIGURE 3

### tNS3 COORDINATES   (Complex A)

| | | Atom Type | Resid | # | X | Y | Z | OCC | B |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | VAL | 1055 | 94.186 | 42.391 | 51.819 | 1.00 | 32.85 |
| ATOM | 2 | CA | VAL | 1055 | 92.743 | 42.519 | 51.462 | 1.00 | 30.82 |
| ATOM | 3 | CB | VAL | 1055 | 92.435 | 41.883 | 50.083 | 1.00 | 30.41 |
| ATOM | 4 | CG1 | VAL | 1055 | 90.953 | 41.986 | 49.767 | 1.00 | 31.38 |
| ATOM | 5 | CG2 | VAL | 1055 | 93.232 | 42.576 | 48.999 | 1.00 | 30.52 |
| ATOM | 6 | C | VAL | 1055 | 91.928 | 41.817 | 52.527 | 1.00 | 30.32 |
| ATOM | 7 | O | VAL | 1055 | 92.271 | 40.715 | 52.954 | 1.00 | 31.39 |
| ATOM | 8 | N | GLU | 1056 | 90.869 | 42.481 | 52.975 | 1.00 | 30.38 |
| ATOM | 9 | CA | GLU | 1056 | 89.985 | 41.933 | 53.994 | 1.00 | 28.82 |
| ATOM | 10 | CB | GLU | 1056 | 89.909 | 42.877 | 55.191 | 1.00 | 28.56 |
| ATOM | 11 | CG | GLU | 1056 | 91.249 | 43.090 | 55.856 | 1.00 | 33.65 |
| ATOM | 12 | CD | GLU | 1056 | 91.183 | 44.066 | 57.007 | 1.00 | 37.88 |
| ATOM | 13 | OE1 | GLU | 1056 | 91.610 | 43.695 | 58.120 | 1.00 | 40.68 |
| ATOM | 14 | OE2 | GLU | 1056 | 90.713 | 45.204 | 56.796 | 1.00 | 40.04 |
| ATOM | 15 | C | GLU | 1056 | 88.590 | 41.675 | 53.442 | 1.00 | 26.54 |
| ATOM | 16 | O | GLU | 1056 | 88.102 | 42.417 | 52.591 | 1.00 | 26.63 |
| ATOM | 17 | N | GLY | 1057 | 87.970 | 40.602 | 53.914 | 1.00 | 24.45 |
| ATOM | 18 | CA | GLY | 1057 | 86.633 | 40.261 | 53.478 | 1.00 | 22.13 |
| ATOM | 19 | C | GLY | 1057 | 85.614 | 40.570 | 54.553 | 1.00 | 21.95 |
| ATOM | 20 | O | GLY | 1057 | 85.918 | 40.510 | 55.742 | 1.00 | 23.57 |
| ATOM | 21 | N | GLU | 1058 | 84.406 | 40.924 | 54.140 | 1.00 | 20.53 |
| ATOM | 22 | CA | GLU | 1058 | 83.352 | 41.236 | 55.084 | 1.00 | 18.51 |
| ATOM | 23 | CB | GLU | 1058 | 82.408 | 42.295 | 54.514 | 1.00 | 18.38 |
| ATOM | 24 | CG | GLU | 1058 | 83.060 | 43.597 | 54.096 | 1.00 | 18.99 |
| ATOM | 25 | CD | GLU | 1058 | 83.531 | 43.593 | 52.650 | 1.00 | 23.27 |
| ATOM | 26 | OE1 | GLU | 1058 | 83.746 | 42.504 | 52.083 | 1.00 | 24.96 |
| ATOM | 27 | OE2 | GLU | 1058 | 83.701 | 44.686 | 52.067 | 1.00 | 26.97 |
| ATOM | 28 | C | GLU | 1058 | 82.580 | 39.954 | 55.338 | 1.00 | 19.61 |
| ATOM | 29 | O | GLU | 1058 | 81.988 | 39.770 | 56.399 | 1.00 | 21.48 |
| ATOM | 30 | N | VAL | 1059 | 82.604 | 39.062 | 54.354 | 1.00 | 18.78 |
| ATOM | 31 | CA | VAL | 1059 | 81.899 | 37.789 | 54.428 | 1.00 | 18.22 |
| ATOM | 32 | CB | VAL | 1059 | 80.990 | 37.583 | 53.170 | 1.00 | 16.33 |
| ATOM | 33 | CG1 | VAL | 1059 | 80.286 | 36.249 | 53.225 | 1.00 | 13.76 |
| ATOM | 34 | CG2 | VAL | 1059 | 79.977 | 38.702 | 53.048 | 1.00 | 12.68 |
| ATOM | 35 | C | VAL | 1059 | 82.903 | 36.644 | 54.491 | 1.00 | 20.89 |
| ATOM | 36 | O | VAL | 1059 | 83.826 | 36.571 | 53.676 | 1.00 | 20.81 |
| ATOM | 37 | N | GLN | 1060 | 82.737 | 35.758 | 55.465 | 1.00 | 21.48 |
| ATOM | 38 | CA | GLN | 1060 | 83.629 | 34.620 | 55.582 | 1.00 | 22.32 |
| ATOM | 39 | CB | GLN | 1060 | 84.405 | 34.633 | 56.908 | 1.00 | 23.40 |
| ATOM | 40 | CG | GLN | 1060 | 83.662 | 35.176 | 58.104 | 1.00 | 24.97 |
| ATOM | 41 | CD | GLN | 1060 | 83.707 | 36.692 | 58.201 | 1.00 | 25.79 |
| ATOM | 42 | OE1 | GLN | 1060 | 84.519 | 37.351 | 57.553 | 1.00 | 27.09 |
| ATOM | 43 | NE2 | GLN | 1060 | 82.842 | 37.252 | 59.031 | 1.00 | 25.24 |
| ATOM | 44 | C | GLN | 1060 | 82.863 | 33.325 | 55.410 | 1.00 | 23.40 |
| ATOM | 45 | O | GLN | 1060 | 81.735 | 33.202 | 55.880 | 1.00 | 25.77 |

## FIGURE 3 (CONT.)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 46 | N | ILE | 1061 | 83.457 | 32.399 | 54.663 | 1.00 | 23.80 |
| ATOM | 47 | CA | ILE | 1061 | 82.882 | 31.086 | 54.390 | 1.00 | 23.08 |
| ATOM | 48 | CB | ILE | 1061 | 83.399 | 30.530 | 53.052 | 1.00 | 23.13 |
| ATOM | 49 | CG2 | ILE | 1061 | 82.659 | 29.258 | 52.698 | 1.00 | 20.59 |
| ATOM | 50 | CG1 | ILE | 1061 | 83.219 | 31.584 | 51.951 | 1.00 | 23.17 |
| ATOM | 51 | CD1 | ILE | 1061 | 83.949 | 31.275 | 50.692 | 1.00 | 21.52 |
| ATOM | 52 | C | ILE | 1061 | 83.335 | 30.173 | 55.517 | 1.00 | 24.42 |
| ATOM | 53 | O | ILE | 1061 | 84.498 | 29.766 | 55.574 | 1.00 | 26.06 |
| ATOM | 54 | N | VAL | 1062 | 82.404 | 29.850 | 56.404 | 1.00 | 25.24 |
| ATOM | 55 | CA | VAL | 1062 | 82.688 | 29.028 | 57.569 | 1.00 | 24.13 |
| ATOM | 56 | CB | VAL | 1062 | 82.085 | 29.682 | 58.832 | 1.00 | 21.93 |
| ATOM | 57 | CG1 | VAL | 1062 | 82.568 | 31.124 | 58.951 | 1.00 | 20.61 |
| ATOM | 58 | CG2 | VAL | 1062 | 80.578 | 29.645 | 58.778 | 1.00 | 18.03 |
| ATOM | 59 | C | VAL | 1062 | 82.201 | 27.587 | 57.443 | 1.00 | 26.46 |
| ATOM | 60 | O | VAL | 1062 | 81.391 | 27.261 | 56.573 | 1.00 | 26.50 |
| ATOM | 61 | N | SER | 1063 | 82.685 | 26.730 | 58.332 | 1.00 | 28.27 |
| ATOM | 62 | CA | SER | 1063 | 82.312 | 25.326 | 58.316 | 1.00 | 29.40 |
| ATOM | 63 | CB | SER | 1063 | 83.246 | 24.539 | 57.389 | 1.00 | 29.43 |
| ATOM | 64 | OG | SER | 1063 | 83.164 | 25.013 | 56.054 | 1.00 | 33.51 |
| ATOM | 65 | C | SER | 1063 | 82.339 | 24.684 | 59.696 | 1.00 | 31.16 |
| ATOM | 66 | O | SER | 1063 | 83.000 | 25.167 | 60.623 | 1.00 | 30.35 |
| ATOM | 67 | N | THR | 1064 | 81.593 | 23.593 | 59.811 | 1.00 | 33.89 |
| ATOM | 68 | CA | THR | 1064 | 81.497 | 22.790 | 61.023 | 1.00 | 33.81 |
| ATOM | 69 | CB | THR | 1064 | 80.091 | 22.855 | 61.651 | 1.00 | 31.40 |
| ATOM | 70 | OG1 | THR | 1064 | 79.099 | 22.536 | 60.664 | 1.00 | 33.92 |
| ATOM | 71 | CG2 | THR | 1064 | 79.825 | 24.230 | 62.216 | 1.00 | 29.94 |
| ATOM | 72 | C | THR | 1064 | 81.769 | 21.383 | 60.511 | 1.00 | 35.92 |
| ATOM | 73 | O | THR | 1064 | 81.951 | 21.200 | 59.305 | 1.00 | 36.71 |
| ATOM | 74 | N | ALA | 1065 | 81.800 | 20.395 | 61.396 | 1.00 | 38.38 |
| ATOM | 75 | CA | ALA | 1065 | 82.060 | 19.022 | 60.975 | 1.00 | 40.41 |
| ATOM | 76 | CB | ALA | 1065 | 82.104 | 18.114 | 62.181 | 1.00 | 41.57 |
| ATOM | 77 | C | ALA | 1065 | 81.044 | 18.490 | 59.966 | 1.00 | 41.85 |
| ATOM | 78 | O | ALA | 1065 | 81.357 | 17.623 | 59.151 | 1.00 | 41.76 |
| ATOM | 79 | N | THR | 1066 | 79.827 | 19.016 | 60.025 | 1.00 | 43.16 |
| ATOM | 80 | CA | THR | 1066 | 78.758 | 18.559 | 59.148 | 1.00 | 45.82 |
| ATOM | 81 | CB | THR | 1066 | 77.582 | 18.022 | 60.003 | 1.00 | 48.55 |
| ATOM | 82 | OG1 | THR | 1066 | 77.141 | 19.047 | 60.914 | 1.00 | 51.57 |
| ATOM | 83 | CG2 | THR | 1066 | 78.009 | 16.795 | 60.791 | 1.00 | 51.00 |
| ATOM | 84 | C | THR | 1066 | 78.147 | 19.613 | 58.224 | 1.00 | 46.64 |
| ATOM | 85 | O | THR | 1066 | 77.374 | 19.265 | 57.323 | 1.00 | 48.12 |
| ATOM | 86 | N | GLN | 1067 | 78.466 | 20.887 | 58.431 | 1.00 | 45.58 |
| ATOM | 87 | CA | GLN | 1067 | 77.829 | 21.923 | 57.636 | 1.00 | 43.33 |
| ATOM | 88 | CB | GLN | 1067 | 76.635 | 22.429 | 58.438 | 1.00 | 44.54 |
| ATOM | 89 | CG | GLN | 1067 | 75.606 | 23.244 | 57.682 | 1.00 | 48.92 |
| ATOM | 90 | CD | GLN | 1067 | 74.377 | 23.595 | 58.535 | 1.00 | 51.71 |
| ATOM | 91 | OE1 | GLN | 1067 | 73.519 | 24.380 | 58.113 | 1.00 | 53.17 |
| ATOM | 92 | NE2 | GLN | 1067 | 74.297 | 23.023 | 59.738 | 1.00 | 49.37 |
| ATOM | 93 | C | GLN | 1067 | 78.720 | 23.091 | 57.269 | 1.00 | 40.47 |
| ATOM | 94 | O | GLN | 1067 | 79.567 | 23.498 | 58.053 | 1.00 | 41.29 |
| ATOM | 95 | N | THR | 1068 | 78.523 | 23.612 | 56.063 | 1.00 | 37.11 |
| ATOM | 96 | CA | THR | 1068 | 79.261 | 24.767 | 55.574 | 1.00 | 30.70 |

FIGURE 3 (CONT.)

| | | | | | | | | | |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 97 | CB | THR | 1068 | 80.113 | 24.436 | 54.331 | 1.00 | 29.76 |
| ATOM | 98 | OG1 | THR | 1068 | 81.008 | 25.521 | 54.062 | 1.00 | 30.04 |
| ATOM | 99 | CG2 | THR | 1068 | 79.241 | 24.184 | 53.113 | 1.00 | 30.99 |
| ATOM | 100 | C | THR | 1068 | 78.236 | 25.843 | 55.234 | 1.00 | 28.68 |
| ATOM | 101 | O | THR | 1068 | 77.192 | 25.565 | 54.644 | 1.00 | 27.99 |
| ATOM | 102 | N | PHE | 1069 | 78.517 | 27.063 | 55.659 | 1.00 | 26.46 |
| ATOM | 103 | CA | PHE | 1069 | 77.631 | 28.186 | 55.420 | 1.00 | 23.03 |
| ATOM | 104 | CB | PHE | 1069 | 76.499 | 28.199 | 56.450 | 1.00 | 22.57 |
| ATOM | 105 | CG | PHE | 1069 | 76.955 | 27.964 | 57.854 | 1.00 | 22.39 |
| ATOM | 106 | CD1 | PHE | 1069 | 77.011 | 29.014 | 58.759 | 1.00 | 22.57 |
| ATOM | 107 | CD2 | PHE | 1069 | 77.351 | 26.699 | 58.271 | 1.00 | 22.33 |
| ATOM | 108 | CE1 | PHE | 1069 | 77.458 | 28.808 | 60.057 | 1.00 | 23.82 |
| ATOM | 109 | CE2 | PHE | 1069 | 77.800 | 26.485 | 59.566 | 1.00 | 22.79 |
| ATOM | 110 | CZ | PHE | 1069 | 77.855 | 27.543 | 60.461 | 1.00 | 23.30 |
| ATOM | 111 | C | PHE | 1069 | 78.456 | 29.472 | 55.447 | 1.00 | 22.55 |
| ATOM | 112 | O | PHE | 1069 | 79.670 | 29.421 | 55.249 | 1.00 | 21.97 |
| ATOM | 113 | N | LEU | 1070 | 77.832 | 30.607 | 55.734 | 1.00 | 19.95 |
| ATOM | 114 | CA | LEU | 1070 | 78.562 | 31.866 | 55.734 | 1.00 | 19.27 |
| ATOM | 115 | CB | LEU | 1070 | 78.091 | 32.748 | 54.571 | 1.00 | 19.20 |
| ATOM | 116 | CG | LEU | 1070 | 78.060 | 32.230 | 53.135 | 1.00 | 16.10 |
| ATOM | 117 | CD1 | LEU | 1070 | 77.451 | 33.307 | 52.257 | 1.00 | 13.03 |
| ATOM | 118 | CD2 | LEU | 1070 | 79.445 | 31.859 | 52.670 | 1.00 | 15.83 |
| ATOM | 119 | C | LEU | 1070 | 78.347 | 32.649 | 57.009 | 1.00 | 18.16 |
| ATOM | 120 | O | LEU | 1070 | 77.443 | 32.345 | 57.781 | 1.00 | 20.67 |
| ATOM | 121 | N | ALA | 1071 | 79.186 | 33.661 | 57.210 | 1.00 | 16.24 |
| ATOM | 122 | CA | ALA | 1071 | 79.091 | 34.565 | 58.349 | 1.00 | 17.10 |
| ATOM | 123 | CB | ALA | 1071 | 80.142 | 34.249 | 59.377 | 1.00 | 19.06 |
| ATOM | 124 | C | ALA | 1071 | 79.340 | 35.935 | 57.750 | 1.00 | 18.14 |
| ATOM | 125 | O | ALA | 1071 | 79.958 | 36.030 | 56.693 | 1.00 | 19.55 |
| ATOM | 126 | N | THR | 1072 | 78.839 | 36.981 | 58.396 | 1.00 | 17.51 |
| ATOM | 127 | CA | THR | 1072 | 78.999 | 38.345 | 57.909 | 1.00 | 16.67 |
| ATOM | 128 | CB | THR | 1072 | 77.679 | 38.890 | 57.335 | 1.00 | 14.90 |
| ATOM | 129 | OG1 | THR | 1072 | 77.249 | 38.048 | 56.269 | 1.00 | 19.26 |
| ATOM | 130 | CG2 | THR | 1072 | 77.852 | 40.303 | 56.799 | 1.00 | 13.79 |
| ATOM | 131 | C | THR | 1072 | 79.410 | 39.262 | 59.049 | 1.00 | 19.92 |
| ATOM | 132 | O | THR | 1072 | 78.785 | 39.264 | 60.112 | 1.00 | 22.53 |
| ATOM | 133 | N | CYS | 1073 | 80.470 | 40.032 | 58.840 | 1.00 | 20.00 |
| ATOM | 134 | CA | CYS | 1073 | 80.916 | 40.960 | 59.856 | 1.00 | 19.38 |
| ATOM | 135 | CB | CYS | 1073 | 82.388 | 41.267 | 59.691 | 1.00 | 17.15 |
| ATOM | 136 | SG | CYS | 1073 | 83.433 | 39.961 | 60.265 | 1.00 | 21.59 |
| ATOM | 137 | C | CYS | 1073 | 80.144 | 42.240 | 59.705 | 1.00 | 20.61 |
| ATOM | 138 | O | CYS | 1073 | 80.125 | 42.821 | 58.623 | 1.00 | 21.53 |
| ATOM | 139 | N | ILE | 1074 | 79.470 | 42.654 | 60.770 | 1.00 | 23.02 |
| ATOM | 140 | CA | ILE | 1074 | 78.706 | 43.903 | 60.793 | 1.00 | 24.61 |
| ATOM | 141 | CB | ILE | 1074 | 77.189 | 43.676 | 60.592 | 1.00 | 24.97 |
| ATOM | 142 | CG2 | ILE | 1074 | 76.426 | 44.967 | 60.844 | 1.00 | 27.22 |
| ATOM | 143 | CG1 | ILE | 1074 | 76.904 | 43.174 | 59.178 | 1.00 | 23.86 |
| ATOM | 144 | CD1 | ILE | 1074 | 75.491 | 42.685 | 58.985 | 1.00 | 25.93 |
| ATOM | 145 | C | ILE | 1074 | 78.943 | 44.491 | 62.176 | 1.00 | 26.19 |
| ATOM | 146 | O | ILE | 1074 | 78.833 | 43.790 | 63.185 | 1.00 | 28.47 |
| ATOM | 147 | N | ASN | 1075 | 79.320 | 45.760 | 62.222 | 1.00 | 26.56 |

FIGURE 3 (CONT.)

| ATOM | 148 | CA | ASN | 1075 | 79.593 | 46.430 | 63.488 | 1.00 | 27.15 |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 149 | CB | ASN | 1075 | 78.297 | 46.703 | 64.261 | 1.00 | 28.70 |
| ATOM | 150 | CG | ASN | 1075 | 77.415 | 47.756 | 63.592 | 1.00 | 30.77 |
| ATOM | 151 | OD1 | ASN | 1075 | 77.829 | 48.418 | 62.639 | 1.00 | 33.91 |
| ATOM | 152 | ND2 | ASN | 1075 | 76.192 | 47.915 | 64.094 | 1.00 | 30.24 |
| ATOM | 153 | C | ASN | 1075 | 80.599 | 45.671 | 64.368 | 1.00 | 28.13 |
| ATOM | 154 | O | ASN | 1075 | 80.388 | 45.504 | 65.569 | 1.00 | 27.91 |
| ATOM | 155 | N | GLY | 1076 | 81.687 | 45.206 | 63.760 | 1.00 | 28.00 |
| ATOM | 156 | CA | GLY | 1076 | 82.723 | 44.506 | 64.502 | 1.00 | 27.37 |
| ATOM | 157 | C | GLY | 1076 | 82.411 | 43.101 | 64.970 | 1.00 | 29.01 |
| ATOM | 158 | O | GLY | 1076 | 83.264 | 42.433 | 65.567 | 1.00 | 28.27 |
| ATOM | 159 | N | VAL | 1077 | 81.205 | 42.631 | 64.678 | 1.00 | 29.05 |
| ATOM | 160 | CA | VAL | 1077 | 80.801 | 41.298 | 65.084 | 1.00 | 27.37 |
| ATOM | 161 | CB | VAL | 1077 | 79.453 | 41.339 | 65.821 | 1.00 | 26.61 |
| ATOM | 162 | CG1 | VAL | 1077 | 79.062 | 39.956 | 66.292 | 1.00 | 27.45 |
| ATOM | 163 | CG2 | VAL | 1077 | 79.536 | 42.281 | 66.995 | 1.00 | 27.61 |
| ATOM | 164 | C | VAL | 1077 | 80.688 | 40.392 | 63.864 | 1.00 | 27.94 |
| ATOM | 165 | O | VAL | 1077 | 80.387 | 40.852 | 62.759 | 1.00 | 29.66 |
| ATOM | 166 | N | CYS | 1078 | 80.989 | 39.114 | 64.062 | 1.00 | 26.17 |
| ATOM | 167 | CA | CYS | 1078 | 80.910 | 38.114 | 63.011 | 1.00 | 23.77 |
| ATOM | 168 | CB | CYS | 1078 | 82.097 | 37.158 | 63.101 | 1.00 | 23.73 |
| ATOM | 169 | SG | CYS | 1078 | 82.221 | 35.981 | 61.746 | 1.00 | 23.84 |
| ATOM | 170 | C | CYS | 1078 | 79.610 | 37.378 | 63.286 | 1.00 | 23.02 |
| ATOM | 171 | O | CYS | 1078 | 79.533 | 36.557 | 64.200 | 1.00 | 24.11 |
| ATOM | 172 | N | TRP | 1079 | 78.576 | 37.726 | 62.534 | 1.00 | 21.24 |
| ATOM | 173 | CA | TRP | 1079 | 77.260 | 37.133 | 62.698 | 1.00 | 19.55 |
| ATOM | 174 | CB | TRP | 1079 | 76.187 | 38.178 | 62.406 | 1.00 | 19.32 |
| ATOM | 175 | CG | TRP | 1079 | 76.340 | 39.431 | 63.178 | 1.00 | 21.82 |
| ATOM | 176 | CD2 | TRP | 1079 | 75.766 | 39.721 | 64.460 | 1.00 | 23.32 |
| ATOM | 177 | CE2 | TRP | 1079 | 76.112 | 41.055 | 64.781 | 1.00 | 24.08 |
| ATOM | 178 | CE3 | TRP | 1079 | 74.989 | 38.986 | 65.364 | 1.00 | 21.58 |
| ATOM | 179 | CD1 | TRP | 1079 | 77.003 | 40.560 | 62.788 | 1.00 | 22.05 |
| ATOM | 180 | NE1 | TRP | 1079 | 76.868 | 41.542 | 63.745 | 1.00 | 23.78 |
| ATOM | 181 | CZ2 | TRP | 1079 | 75.703 | 41.670 | 65.967 | 1.00 | 22.89 |
| ATOM | 182 | CZ3 | TRP | 1079 | 74.582 | 39.596 | 66.540 | 1.00 | 22.78 |
| ATOM | 183 | CH2 | TRP | 1079 | 74.940 | 40.929 | 66.831 | 1.00 | 23.44 |
| ATOM | 184 | C | TRP | 1079 | 77.028 | 35.976 | 61.763 | 1.00 | 18.27 |
| ATOM | 185 | O | TRP | 1079 | 77.576 | 35.939 | 60.661 | 1.00 | 20.23 |
| ATOM | 186 | N | THR | 1080 | 76.196 | 35.041 | 62.200 | 1.00 | 17.65 |
| ATOM | 187 | CA | THR | 1080 | 75.813 | 33.895 | 61.391 | 1.00 | 18.57 |
| ATOM | 188 | CB | THR | 1080 | 76.917 | 32.826 | 61.319 | 1.00 | 18.31 |
| ATOM | 189 | OG1 | THR | 1080 | 76.535 | 31.806 | 60.384 | 1.00 | 15.58 |
| ATOM | 190 | CG2 | THR | 1080 | 77.164 | 32.212 | 62.666 | 1.00 | 16.32 |
| ATOM | 191 | C | THR | 1080 | 74.506 | 33.321 | 61.930 | 1.00 | 19.72 |
| ATOM | 192 | O | THR | 1080 | 73.939 | 33.844 | 62.894 | 1.00 | 20.69 |
| ATOM | 193 | N | VAL | 1081 | 74.023 | 32.258 | 61.304 | 1.00 | 22.55 |
| ATOM | 194 | CA | VAL | 1081 | 72.767 | 31.633 | 61.700 | 1.00 | 23.39 |
| ATOM | 195 | CB | VAL | 1081 | 72.019 | 31.058 | 60.473 | 1.00 | 21.81 |
| ATOM | 196 | CG1 | VAL | 1081 | 71.432 | 32.176 | 59.648 | 1.00 | 19.45 |
| ATOM | 197 | CG2 | VAL | 1081 | 72.972 | 30.227 | 59.617 | 1.00 | 22.36 |
| ATOM | 198 | C | VAL | 1081 | 72.942 | 30.524 | 62.729 | 1.00 | 25.42 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 199 | O | VAL | 1081 | 73.693 | 29.565 | 62.510 | 1.00 | 27.35 |
| ATOM | 200 | N | TYR | 1082 | 72.191 | 30.632 | 63.823 | 1.00 | 27.30 |
| ATOM | 201 | CA | TYR | 1082 | 72.211 | 29.644 | 64.902 | 1.00 | 28.71 |
| ATOM | 202 | CB | TYR | 1082 | 71.139 | 29.964 | 65.946 | 1.00 | 29.28 |
| ATOM | 203 | CG | TYR | 1082 | 71.171 | 29.063 | 67.161 | 1.00 | 29.31 |
| ATOM | 204 | CD1 | TYR | 1082 | 70.439 | 27.883 | 67.191 | 1.00 | 32.22 |
| ATOM | 205 | CE1 | TYR | 1082 | 70.458 | 27.048 | 68.308 | 1.00 | 35.00 |
| ATOM | 206 | CD2 | TYR | 1082 | 71.928 | 29.395 | 68.281 | 1.00 | 29.57 |
| ATOM | 207 | CE2 | TYR | 1082 | 71.957 | 28.570 | 69.406 | 1.00 | 32.16 |
| ATOM | 208 | CZ | TYR | 1082 | 71.216 | 27.395 | 69.415 | 1.00 | 34.16 |
| ATOM | 209 | OH | TYR | 1082 | 71.214 | 26.568 | 70.524 | 1.00 | 34.78 |
| ATOM | 210 | C | TYR | 1082 | 72.005 | 28.218 | 64.398 | 1.00 | 28.97 |
| ATOM | 211 | O | TYR | 1082 | 72.591 | 27.286 | 64.945 | 1.00 | 31.64 |
| ATOM | 212 | N | HIS | 1083 | 71.200 | 28.046 | 63.350 | 1.00 | 28.60 |
| ATOM | 213 | CA | HIS | 1083 | 70.943 | 26.717 | 62.800 | 1.00 | 29.08 |
| ATOM | 214 | CB | HIS | 1083 | 69.730 | 26.725 | 61.858 | 1.00 | 28.98 |
| ATOM | 215 | CG | HIS | 1083 | 69.984 | 27.333 | 60.508 | 1.00 | 27.71 |
| ATOM | 216 | CD2 | HIS | 1083 | 70.696 | 26.886 | 59.443 | 1.00 | 27.80 |
| ATOM | 217 | ND1 | HIS | 1083 | 69.392 | 28.509 | 60.106 | 1.00 | 26.55 |
| ATOM | 218 | CE1 | HIS | 1083 | 69.724 | 28.766 | 58.852 | 1.00 | 28.23 |
| ATOM | 219 | NE2 | HIS | 1083 | 70.514 | 27.795 | 58.427 | 1.00 | 28.18 |
| ATOM | 220 | C | HIS | 1083 | 72.153 | 26.103 | 62.102 | 1.00 | 31.61 |
| ATOM | 221 | O | HIS | 1083 | 72.056 | 25.016 | 61.516 | 1.00 | 32.83 |
| ATOM | 222 | N | GLY | 1084 | 73.270 | 26.826 | 62.110 | 1.00 | 31.35 |
| ATOM | 223 | CA | GLY | 1084 | 74.479 | 26.329 | 61.486 | 1.00 | 30.49 |
| ATOM | 224 | C | GLY | 1084 | 75.597 | 26.297 | 62.501 | 1.00 | 30.79 |
| ATOM | 225 | O | GLY | 1084 | 76.345 | 25.322 | 62.586 | 1.00 | 31.01 |
| ATOM | 226 | N | ALA | 1085 | 75.710 | 27.364 | 63.281 | 1.00 | 29.67 |
| ATOM | 227 | CA | ALA | 1085 | 76.756 | 27.463 | 64.291 | 1.00 | 29.18 |
| ATOM | 228 | CB | ALA | 1085 | 77.102 | 28.919 | 64.538 | 1.00 | 27.13 |
| ATOM | 229 | C | ALA | 1085 | 76.385 | 26.797 | 65.608 | 1.00 | 30.86 |
| ATOM | 230 | O | ALA | 1085 | 77.229 | 26.191 | 66.266 | 1.00 | 32.83 |
| ATOM | 231 | N | GLY | 1086 | 75.120 | 26.912 | 65.996 | 1.00 | 31.95 |
| ATOM | 232 | CA | GLY | 1086 | 74.691 | 26.347 | 67.259 | 1.00 | 30.00 |
| ATOM | 233 | C | GLY | 1086 | 75.280 | 27.240 | 68.329 | 1.00 | 30.52 |
| ATOM | 234 | O | GLY | 1086 | 75.093 | 28.456 | 68.288 | 1.00 | 31.56 |
| ATOM | 235 | N | THR | 1087 | 76.004 | 26.659 | 69.277 | 1.00 | 29.74 |
| ATOM | 236 | CA | THR | 1087 | 76.632 | 27.445 | 70.334 | 1.00 | 29.99 |
| ATOM | 237 | CB | THR | 1087 | 76.202 | 26.964 | 71.722 | 1.00 | 31.53 |
| ATOM | 238 | OG1 | THR | 1087 | 76.282 | 25.531 | 71.779 | 1.00 | 33.33 |
| ATOM | 239 | CG2 | THR | 1087 | 74.792 | 27.428 | 72.043 | 1.00 | 32.33 |
| ATOM | 240 | C | THR | 1087 | 78.138 | 27.277 | 70.235 | 1.00 | 29.06 |
| ATOM | 241 | O | THR | 1087 | 78.863 | 27.526 | 71.195 | 1.00 | 29.33 |
| ATOM | 242 | N | ARG | 1088 | 78.602 | 26.848 | 69.068 | 1.00 | 27.32 |
| ATOM | 243 | CA | ARG | 1088 | 80.013 | 26.607 | 68.849 | 1.00 | 25.61 |
| ATOM | 244 | CB | ARG | 1088 | 80.232 | 25.970 | 67.484 | 1.00 | 24.43 |
| ATOM | 245 | CG | ARG | 1088 | 79.894 | 24.510 | 67.450 | 1.00 | 24.44 |
| ATOM | 246 | CD | ARG | 1088 | 79.804 | 24.007 | 66.034 | 1.00 | 26.01 |
| ATOM | 247 | NE | ARG | 1088 | 78.457 | 23.542 | 65.721 | 1.00 | 25.14 |
| ATOM | 248 | CZ | ARG | 1088 | 78.181 | 22.324 | 65.274 | 1.00 | 27.41 |
| ATOM | 249 | NH1 | ARG | 1088 | 79.162 | 21.449 | 65.099 | 1.00 | 29.46 |

FIGURE 3 (CONT.)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 250 | NH2 | ARG | 1088 | 76.937 | 21.999 | 64.942 | 1.00 | 27.99 |
| ATOM | 251 | C | ARG | 1088 | 80.880 | 27.837 | 68.974 | 1.00 | 26.13 |
| ATOM | 252 | O | ARG | 1088 | 80.407 | 28.963 | 68.843 | 1.00 | 27.98 |
| ATOM | 253 | N | THR | 1089 | 82.145 | 27.598 | 69.294 | 1.00 | 25.72 |
| ATOM | 254 | CA | THR | 1089 | 83.135 | 28.648 | 69.412 | 1.00 | 24.74 |
| ATOM | 255 | CB | THR | 1089 | 84.295 | 28.219 | 70.320 | 1.00 | 21.05 |
| ATOM | 256 | OG1 | THR | 1089 | 84.682 | 26.880 | 69.991 | 1.00 | 21.01 |
| ATOM | 257 | CG2 | THR | 1089 | 83.908 | 28.296 | 71.765 | 1.00 | 21.52 |
| ATOM | 258 | C | THR | 1089 | 83.699 | 28.785 | 68.012 | 1.00 | 25.12 |
| ATOM | 259 | O | THR | 1089 | 83.616 | 27.844 | 67.218 | 1.00 | 27.12 |
| ATOM | 260 | N | ILE | 1090 | 84.252 | 29.944 | 67.694 | 1.00 | 23.10 |
| ATOM | 261 | CA | ILE | 1090 | 84.854 | 30.135 | 66.392 | 1.00 | 22.50 |
| ATOM | 262 | CB | ILE | 1090 | 84.540 | 31.546 | 65.840 | 1.00 | 21.33 |
| ATOM | 263 | CG2 | ILE | 1090 | 85.167 | 32.617 | 66.699 | 1.00 | 20.09 |
| ATOM | 264 | CG1 | ILE | 1090 | 84.962 | 31.653 | 64.378 | 1.00 | 20.03 |
| ATOM | 265 | CD1 | ILE | 1090 | 84.429 | 32.877 | 63.701 | 1.00 | 19.81 |
| ATOM | 266 | C | ILE | 1090 | 86.358 | 29.896 | 66.581 | 1.00 | 24.31 |
| ATOM | 267 | O | ILE | 1090 | 86.924 | 30.289 | 67.611 | 1.00 | 25.80 |
| ATOM | 268 | N | ALA | 1091 | 86.981 | 29.177 | 65.649 | 1.00 | 23.50 |
| ATOM | 269 | CA | ALA | 1091 | 88.412 | 28.883 | 65.728 | 1.00 | 23.75 |
| ATOM | 270 | CB | ALA | 1091 | 88.797 | 27.871 | 64.670 | 1.00 | 22.92 |
| ATOM | 271 | C | ALA | 1091 | 89.267 | 30.147 | 65.589 | 1.00 | 25.79 |
| ATOM | 272 | O | ALA | 1091 | 88.962 | 31.039 | 64.789 | 1.00 | 27.65 |
| ATOM | 273 | N | SER | 1092 | 90.354 | 30.201 | 66.349 | 1.00 | 25.22 |
| ATOM | 274 | CA | SER | 1092 | 91.271 | 31.335 | 66.345 | 1.00 | 24.64 |
| ATOM | 275 | CB | SER | 1092 | 90.898 | 32.264 | 67.501 | 1.00 | 24.34 |
| ATOM | 276 | OG | SER | 1092 | 91.981 | 33.043 | 67.962 | 1.00 | 27.32 |
| ATOM | 277 | C | SER | 1092 | 92.686 | 30.778 | 66.518 | 1.00 | 26.18 |
| ATOM | 278 | O | SER | 1092 | 92.859 | 29.722 | 67.129 | 1.00 | 28.18 |
| ATOM | 279 | N | PRO | 1093 | 93.712 | 31.449 | 65.953 | 1.00 | 26.97 |
| ATOM | 280 | CD | PRO | 1093 | 93.667 | 32.638 | 65.084 | 1.00 | 27.37 |
| ATOM | 281 | CA | PRO | 1093 | 95.094 | 30.955 | 66.092 | 1.00 | 27.58 |
| ATOM | 282 | CB | PRO | 1093 | 95.888 | 31.857 | 65.133 | 1.00 | 26.90 |
| ATOM | 283 | CG | PRO | 1093 | 95.105 | 33.123 | 65.128 | 1.00 | 28.05 |
| ATOM | 284 | C | PRO | 1093 | 95.618 | 31.011 | 67.533 | 1.00 | 27.01 |
| ATOM | 285 | O | PRO | 1093 | 96.778 | 30.729 | 67.803 | 1.00 | 25.78 |
| ATOM | 286 | N | LYS | 1094 | 94.742 | 31.398 | 68.447 | 1.00 | 28.06 |
| ATOM | 287 | CA | LYS | 1094 | 95.060 | 31.469 | 69.858 | 1.00 | 29.03 |
| ATOM | 288 | CB | LYS | 1094 | 94.935 | 32.901 | 70.355 | 1.00 | 27.19 |
| ATOM | 289 | CG | LYS | 1094 | 96.041 | 33.832 | 69.933 | 1.00 | 30.62 |
| ATOM | 290 | CD | LYS | 1094 | 95.763 | 35.182 | 70.569 | 1.00 | 34.13 |
| ATOM | 291 | CE | LYS | 1094 | 96.891 | 36.178 | 70.407 | 1.00 | 36.40 |
| ATOM | 292 | NZ | LYS | 1094 | 96.526 | 37.422 | 71.149 | 1.00 | 40.35 |
| ATOM | 293 | C | LYS | 1094 | 94.058 | 30.599 | 70.617 | 1.00 | 29.44 |
| ATOM | 294 | O | LYS | 1094 | 93.960 | 30.680 | 71.842 | 1.00 | 30.88 |
| ATOM | 295 | N | GLY | 1095 | 93.298 | 29.787 | 69.889 | 1.00 | 30.20 |
| ATOM | 296 | CA | GLY | 1095 | 92.310 | 28.930 | 70.523 | 1.00 | 30.19 |
| ATOM | 297 | C | GLY | 1095 | 90.878 | 29.342 | 70.217 | 1.00 | 29.06 |
| ATOM | 298 | O | GLY | 1095 | 90.654 | 30.374 | 69.580 | 1.00 | 28.17 |
| ATOM | 299 | N | PRO | 1096 | 89.882 | 28.553 | 70.660 | 1.00 | 28.19 |
| ATOM | 300 | CD | PRO | 1096 | 90.042 | 27.313 | 71.439 | 1.00 | 26.15 |

FIGURE 3 (CONT.)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 301 | CA | PRO | 1096 | 88.461 | 28.827 | 70.433 | 1.00 | 27.36 |
| ATOM | 302 | CB | PRO | 1096 | 87.780 | 27.625 | 71.083 | 1.00 | 27.13 |
| ATOM | 303 | CG | PRO | 1096 | 88.735 | 27.236 | 72.166 | 1.00 | 24.95 |
| ATOM | 304 | C | PRO | 1096 | 87.977 | 30.124 | 71.047 | 1.00 | 26.27 |
| ATOM | 305 | O | PRO | 1096 | 88.301 | 30.430 | 72.194 | 1.00 | 27.96 |
| ATOM | 306 | N | VAL | 1097 | 87.173 | 30.862 | 70.294 | 1.00 | 24.47 |
| ATOM | 307 | CA | VAL | 1097 | 86.627 | 32.130 | 70.755 | 1.00 | 24.49 |
| ATOM | 308 | CB | VAL | 1097 | 86.875 | 33.243 | 69.719 | 1.00 | 22.40 |
| ATOM | 309 | CG1 | VAL | 1097 | 86.522 | 34.605 | 70.300 | 1.00 | 20.17 |
| ATOM | 310 | CG2 | VAL | 1097 | 88.314 | 33.214 | 69.269 | 1.00 | 20.81 |
| ATOM | 311 | C | VAL | 1097 | 85.131 | 31.928 | 70.937 | 1.00 | 25.90 |
| ATOM | 312 | O | VAL | 1097 | 84.464 | 31.381 | 70.065 | 1.00 | 27.10 |
| ATOM | 313 | N | ILE | 1098 | 84.598 | 32.365 | 72.066 | 1.00 | 27.33 |
| ATOM | 314 | CA | ILE | 1098 | 83.182 | 32.179 | 72.326 | 1.00 | 28.53 |
| ATOM | 315 | CB | ILE | 1098 | 82.905 | 31.988 | 73.815 | 1.00 | 28.58 |
| ATOM | 316 | CG2 | ILE | 1098 | 83.811 | 30.911 | 74.360 | 1.00 | 27.94 |
| ATOM | 317 | CG1 | ILE | 1098 | 83.120 | 33.299 | 74.568 | 1.00 | 30.72 |
| ATOM | 318 | CD1 | ILE | 1098 | 82.509 | 33.302 | 75.955 | 1.00 | 34.23 |
| ATOM | 319 | C | ILE | 1098 | 82.278 | 33.277 | 71.785 | 1.00 | 29.52 |
| ATOM | 320 | O | ILE | 1098 | 82.671 | 34.441 | 71.676 | 1.00 | 29.80 |
| ATOM | 321 | N | GLN | 1099 | 81.050 | 32.886 | 71.471 | 1.00 | 29.40 |
| ATOM | 322 | CA | GLN | 1099 | 80.064 | 33.804 | 70.933 | 1.00 | 28.62 |
| ATOM | 323 | CB | GLN | 1099 | 78.738 | 33.078 | 70.717 | 1.00 | 26.55 |
| ATOM | 324 | CG | GLN | 1099 | 78.850 | 31.815 | 69.887 | 1.00 | 23.75 |
| ATOM | 325 | CD | GLN | 1099 | 77.506 | 31.260 | 69.498 | 1.00 | 23.24 |
| ATOM | 326 | OE1 | GLN | 1099 | 76.475 | 31.676 | 70.018 | 1.00 | 24.67 |
| ATOM | 327 | NE2 | GLN | 1099 | 77.507 | 30.317 | 68.570 | 1.00 | 25.50 |
| ATOM | 328 | C | GLN | 1099 | 79.842 | 34.976 | 71.865 | 1.00 | 29.81 |
| ATOM | 329 | O | GLN | 1099 | 79.799 | 34.803 | 73.081 | 1.00 | 30.77 |
| ATOM | 330 | N | MET | 1100 | 79.802 | 36.175 | 71.293 | 1.00 | 30.86 |
| ATOM | 331 | CA | MET | 1100 | 79.545 | 37.388 | 72.057 | 1.00 | 31.65 |
| ATOM | 332 | CB | MET | 1100 | 79.942 | 38.628 | 71.260 | 1.00 | 33.79 |
| ATOM | 333 | CG | MET | 1100 | 81.407 | 38.978 | 71.236 | 1.00 | 36.58 |
| ATOM | 334 | SD | MET | 1100 | 81.638 | 40.325 | 70.061 | 1.00 | 40.15 |
| ATOM | 335 | CE | MET | 1100 | 81.416 | 41.748 | 71.118 | 1.00 | 41.86 |
| ATOM | 336 | C | MET | 1100 | 78.043 | 37.439 | 72.266 | 1.00 | 32.12 |
| ATOM | 337 | O | MET | 1100 | 77.565 | 37.967 | 73.266 | 1.00 | 31.59 |
| ATOM | 338 | N | TYR | 1101 | 77.305 | 36.926 | 71.281 | 1.00 | 32.79 |
| ATOM | 339 | CA | TYR | 1101 | 75.847 | 36.914 | 71.320 | 1.00 | 32.46 |
| ATOM | 340 | CB | TYR | 1101 | 75.277 | 38.034 | 70.446 | 1.00 | 31.02 |
| ATOM | 341 | CG | TYR | 1101 | 75.930 | 39.378 | 70.636 | 1.00 | 31.88 |
| ATOM | 342 | CD1 | TYR | 1101 | 76.961 | 39.795 | 69.792 | 1.00 | 34.30 |
| ATOM | 343 | CE1 | TYR | 1101 | 77.591 | 41.018 | 69.973 | 1.00 | 33.36 |
| ATOM | 344 | CD2 | TYR | 1101 | 75.540 | 40.224 | 71.667 | 1.00 | 30.84 |
| ATOM | 345 | CE2 | TYR | 1101 | 76.162 | 41.446 | 71.857 | 1.00 | 31.48 |
| ATOM | 346 | CZ | TYR | 1101 | 77.186 | 41.833 | 71.008 | 1.00 | 34.27 |
| ATOM | 347 | OH | TYR | 1101 | 77.828 | 43.035 | 71.205 | 1.00 | 40.40 |
| ATOM | 348 | C | TYR | 1101 | 75.300 | 35.593 | 70.802 | 1.00 | 33.51 |
| ATOM | 349 | O | TYR | 1101 | 75.825 | 35.025 | 69.852 | 1.00 | 32.08 |
| ATOM | 350 | N | THR | 1102 | 74.247 | 35.113 | 71.449 | 1.00 | 35.21 |
| ATOM | 351 | CA | THR | 1102 | 73.571 | 33.889 | 71.063 | 1.00 | 36.92 |

| ATOM | 352 | CB  | THR | 1102 | 73.904 | 32.722 | 71.996 | 1.00 | 35.96 |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 353 | OG1 | THR | 1102 | 75.323 | 32.600 | 72.131 | 1.00 | 38.23 |
| ATOM | 354 | CG2 | THR | 1102 | 73.356 | 31.429 | 71.426 | 1.00 | 37.30 |
| ATOM | 355 | C   | THR | 1102 | 72.102 | 34.232 | 71.220 | 1.00 | 39.19 |
| ATOM | 356 | O   | THR | 1102 | 71.663 | 34.661 | 72.292 | 1.00 | 39.17 |
| ATOM | 357 | N   | ASN | 1103 | 71.351 | 34.079 | 70.140 | 1.00 | 42.34 |
| ATOM | 358 | CA  | ASN | 1103 | 69.932 | 34.395 | 70.139 | 1.00 | 45.00 |
| ATOM | 359 | CB  | ASN | 1103 | 69.708 | 35.765 | 69.491 | 1.00 | 47.82 |
| ATOM | 360 | CG  | ASN | 1103 | 68.276 | 36.248 | 69.622 | 1.00 | 50.28 |
| ATOM | 361 | OD1 | ASN | 1103 | 67.325 | 35.471 | 69.499 | 1.00 | 50.88 |
| ATOM | 362 | ND2 | ASN | 1103 | 68.114 | 37.536 | 69.889 | 1.00 | 51.98 |
| ATOM | 363 | C   | ASN | 1103 | 69.198 | 33.315 | 69.356 | 1.00 | 46.48 |
| ATOM | 364 | O   | ASN | 1103 | 68.956 | 33.457 | 68.157 | 1.00 | 47.79 |
| ATOM | 365 | N   | VAL | 1104 | 68.862 | 32.227 | 70.038 | 1.00 | 47.60 |
| ATOM | 366 | CA  | VAL | 1104 | 68.170 | 31.115 | 69.407 | 1.00 | 48.19 |
| ATOM | 367 | CB  | VAL | 1104 | 67.859 | 30.009 | 70.423 | 1.00 | 48.12 |
| ATOM | 368 | CG1 | VAL | 1104 | 67.298 | 28.787 | 69.713 | 1.00 | 48.17 |
| ATOM | 369 | CG2 | VAL | 1104 | 69.120 | 29.646 | 71.196 | 1.00 | 48.35 |
| ATOM | 370 | C   | VAL | 1104 | 66.882 | 31.549 | 68.711 | 1.00 | 49.41 |
| ATOM | 371 | O   | VAL | 1104 | 66.608 | 31.095 | 67.602 | 1.00 | 49.88 |
| ATOM | 372 | N   | ASP | 1105 | 66.115 | 32.437 | 69.343 | 1.00 | 50.15 |
| ATOM | 373 | CA  | ASP | 1105 | 64.856 | 32.921 | 68.770 | 1.00 | 51.06 |
| ATOM | 374 | CB  | ASP | 1105 | 64.190 | 33.946 | 69.697 | 1.00 | 54.26 |
| ATOM | 375 | CG  | ASP | 1105 | 63.123 | 33.329 | 70.588 | 1.00 | 57.62 |
| ATOM | 376 | OD1 | ASP | 1105 | 62.581 | 34.062 | 71.446 | 1.00 | 59.65 |
| ATOM | 377 | OD2 | ASP | 1105 | 62.819 | 32.125 | 70.428 | 1.00 | 59.74 |
| ATOM | 378 | C   | ASP | 1105 | 65.023 | 33.537 | 67.394 | 1.00 | 50.07 |
| ATOM | 379 | O   | ASP | 1105 | 64.264 | 33.238 | 66.467 | 1.00 | 52.01 |
| ATOM | 380 | N   | GLN | 1106 | 66.022 | 34.397 | 67.262 | 1.00 | 47.71 |
| ATOM | 381 | CA  | GLN | 1106 | 66.276 | 35.061 | 65.997 | 1.00 | 45.61 |
| ATOM | 382 | CB  | GLN | 1106 | 66.844 | 36.452 | 66.252 | 1.00 | 47.45 |
| ATOM | 383 | CG  | GLN | 1106 | 65.850 | 37.347 | 66.976 | 1.00 | 52.29 |
| ATOM | 384 | CD  | GLN | 1106 | 66.365 | 38.750 | 67.222 | 1.00 | 54.66 |
| ATOM | 385 | OE1 | GLN | 1106 | 67.565 | 38.964 | 67.405 | 1.00 | 56.39 |
| ATOM | 386 | NE2 | GLN | 1106 | 65.455 | 39.719 | 67.233 | 1.00 | 54.76 |
| ATOM | 387 | C   | GLN | 1106 | 67.161 | 34.281 | 65.034 | 1.00 | 43.29 |
| ATOM | 388 | O   | GLN | 1106 | 67.370 | 34.715 | 63.904 | 1.00 | 44.19 |
| ATOM | 389 | N   | ASP | 1107 | 67.629 | 33.110 | 65.458 | 1.00 | 40.90 |
| ATOM | 390 | CA  | ASP | 1107 | 68.503 | 32.279 | 64.630 | 1.00 | 39.02 |
| ATOM | 391 | CB  | ASP | 1107 | 67.818 | 31.993 | 63.288 | 1.00 | 36.53 |
| ATOM | 392 | CG  | ASP | 1107 | 68.386 | 30.779 | 62.580 | 1.00 | 38.24 |
| ATOM | 393 | OD1 | ASP | 1107 | 69.035 | 29.937 | 63.233 | 1.00 | 39.97 |
| ATOM | 394 | OD2 | ASP | 1107 | 68.156 | 30.655 | 61.363 | 1.00 | 39.42 |
| ATOM | 395 | C   | ASP | 1107 | 69.813 | 33.045 | 64.407 | 1.00 | 38.47 |
| ATOM | 396 | O   | ASP | 1107 | 70.500 | 32.848 | 63.406 | 1.00 | 38.85 |
| ATOM | 397 | N   | LEU | 1108 | 70.192 | 33.845 | 65.400 | 1.00 | 37.86 |
| ATOM | 398 | CA  | LEU | 1108 | 71.369 | 34.702 | 65.316 | 1.00 | 37.42 |
| ATOM | 399 | CB  | LEU | 1108 | 70.901 | 36.155 | 65.431 | 1.00 | 35.72 |
| ATOM | 400 | CG  | LEU | 1108 | 71.902 | 37.299 | 65.315 | 1.00 | 33.41 |
| ATOM | 401 | CD1 | LEU | 1108 | 72.538 | 37.304 | 63.944 | 1.00 | 33.86 |
| ATOM | 402 | CD2 | LEU | 1108 | 71.163 | 38.594 | 65.539 | 1.00 | 35.77 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 403 | C | LEU | 1108 | 72.445 | 34.471 | 66.366 | 1.00 | 37.37 |
| ATOM | 404 | O | LEU | 1108 | 72.145 | 34.391 | 67.558 | 1.00 | 38.07 |
| ATOM | 405 | N | VAL | 1109 | 73.698 | 34.388 | 65.924 | 1.00 | 35.09 |
| ATOM | 406 | CA | VAL | 1109 | 74.830 | 34.228 | 66.838 | 1.00 | 33.17 |
| ATOM | 407 | CB | VAL | 1109 | 75.296 | 32.744 | 67.025 | 1.00 | 32.32 |
| ATOM | 408 | CG1 | VAL | 1109 | 74.117 | 31.841 | 67.272 | 1.00 | 32.33 |
| ATOM | 409 | CG2 | VAL | 1109 | 76.119 | 32.264 | 65.860 | 1.00 | 31.84 |
| ATOM | 410 | C | VAL | 1109 | 75.972 | 35.070 | 66.296 | 1.00 | 31.38 |
| ATOM | 411 | O | VAL | 1109 | 76.080 | 35.272 | 65.087 | 1.00 | 32.93 |
| ATOM | 412 | N | GLY | 1110 | 76.815 | 35.570 | 67.183 | 1.00 | 29.70 |
| ATOM | 413 | CA | GLY | 1110 | 77.917 | 36.394 | 66.743 | 1.00 | 26.58 |
| ATOM | 414 | C | GLY | 1110 | 79.129 | 36.273 | 67.627 | 1.00 | 25.55 |
| ATOM | 415 | O | GLY | 1110 | 79.008 | 36.097 | 68.840 | 1.00 | 25.57 |
| ATOM | 416 | N | TRP | 1111 | 80.300 | 36.317 | 67.004 | 1.00 | 24.66 |
| ATOM | 417 | CA | TRP | 1111 | 81.574 | 36.241 | 67.713 | 1.00 | 23.97 |
| ATOM | 418 | CB | TRP | 1111 | 82.415 | 35.077 | 67.186 | 1.00 | 22.57 |
| ATOM | 419 | CG | TRP | 1111 | 81.754 | 33.720 | 67.136 | 1.00 | 22.78 |
| ATOM | 420 | CD2 | TRP | 1111 | 81.163 | 33.091 | 65.987 | 1.00 | 20.85 |
| ATOM | 421 | CE2 | TRP | 1111 | 80.824 | 31.772 | 66.360 | 1.00 | 19.39 |
| ATOM | 422 | CE3 | TRP | 1111 | 80.906 | 33.510 | 64.674 | 1.00 | 18.90 |
| ATOM | 423 | CD1 | TRP | 1111 | 81.725 | 32.785 | 68.135 | 1.00 | 21.78 |
| ATOM | 424 | NE1 | TRP | 1111 | 81.175 | 31.614 | 67.675 | 1.00 | 21.65 |
| ATOM | 425 | CZ2 | TRP | 1111 | 80.240 | 30.870 | 65.474 | 1.00 | 19.81 |
| ATOM | 426 | CZ3 | TRP | 1111 | 80.324 | 32.613 | 63.790 | 1.00 | 18.79 |
| ATOM | 427 | CH2 | TRP | 1111 | 80.001 | 31.306 | 64.193 | 1.00 | 20.56 |
| ATOM | 428 | C | TRP | 1111 | 82.298 | 37.532 | 67.355 | 1.00 | 25.16 |
| ATOM | 429 | O | TRP | 1111 | 81.788 | 38.321 | 66.563 | 1.00 | 25.20 |
| ATOM | 430 | N | PRO | 1112 | 83.451 | 37.813 | 67.989 | 1.00 | 25.84 |
| ATOM | 431 | CD | PRO | 1112 | 84.090 | 37.167 | 69.149 | 1.00 | 25.27 |
| ATOM | 432 | CA | PRO | 1112 | 84.159 | 39.048 | 67.627 | 1.00 | 24.42 |
| ATOM | 433 | CB | PRO | 1112 | 85.322 | 39.063 | 68.611 | 1.00 | 23.55 |
| ATOM | 434 | CG | PRO | 1112 | 84.768 | 38.329 | 69.801 | 1.00 | 23.65 |
| ATOM | 435 | C | PRO | 1112 | 84.666 | 38.826 | 66.194 | 1.00 | 25.76 |
| ATOM | 436 | O | PRO | 1112 | 84.988 | 37.693 | 65.829 | 1.00 | 27.02 |
| ATOM | 437 | N | ALA | 1113 | 84.697 | 39.863 | 65.366 | 1.00 | 23.75 |
| ATOM | 438 | CA | ALA | 1113 | 85.159 | 39.686 | 63.995 | 1.00 | 22.81 |
| ATOM | 439 | CB | ALA | 1113 | 85.051 | 40.980 | 63.239 | 1.00 | 25.86 |
| ATOM | 440 | C | ALA | 1113 | 86.592 | 39.158 | 63.959 | 1.00 | 23.10 |
| ATOM | 441 | O | ALA | 1113 | 87.491 | 39.730 | 64.567 | 1.00 | 25.15 |
| ATOM | 442 | N | PRO | 1114 | 86.826 | 38.071 | 63.212 | 1.00 | 23.57 |
| ATOM | 443 | CD | PRO | 1114 | 85.827 | 37.384 | 62.375 | 1.00 | 24.85 |
| ATOM | 444 | CA | PRO | 1114 | 88.135 | 37.433 | 63.074 | 1.00 | 24.09 |
| ATOM | 445 | CB | PRO | 1114 | 87.790 | 36.144 | 62.340 | 1.00 | 23.05 |
| ATOM | 446 | CG | PRO | 1114 | 86.691 | 36.587 | 61.430 | 1.00 | 23.55 |
| ATOM | 447 | C | PRO | 1114 | 89.160 | 38.250 | 62.296 | 1.00 | 27.35 |
| ATOM | 448 | O | PRO | 1114 | 88.904 | 39.390 | 61.896 | 1.00 | 28.70 |
| ATOM | 449 | N | GLN | 1115 | 90.324 | 37.654 | 62.078 | 1.00 | 28.98 |
| ATOM | 450 | CA | GLN | 1115 | 91.380 | 38.312 | 61.331 | 1.00 | 32.07 |
| ATOM | 451 | CB | GLN | 1115 | 92.747 | 37.751 | 61.726 | 1.00 | 35.02 |
| ATOM | 452 | CG | GLN | 1115 | 93.188 | 38.161 | 63.107 | 1.00 | 40.55 |
| ATOM | 453 | CD | GLN | 1115 | 94.606 | 37.721 | 63.422 | 1.00 | 43.24 |

FIGURE 3 (CONT.)

| ATOM | 454 | OE1 | GLN | 1115 | 94.851 | 36.571 | 63.793 | 1.00 | 41.11 |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 455 | NE2 | GLN | 1115 | 95.547 | 38.649 | 63.308 | 1.00 | 45.52 |
| ATOM | 456 | C   | GLN | 1115 | 91.168 | 38.171 | 59.821 | 1.00 | 31.93 |
| ATOM | 457 | O   | GLN | 1115 | 90.705 | 37.137 | 59.329 | 1.00 | 30.69 |
| ATOM | 458 | N   | GLY | 1116 | 91.512 | 39.225 | 59.093 | 1.00 | 31.14 |
| ATOM | 459 | CA  | GLY | 1116 | 91.354 | 39.206 | 57.653 | 1.00 | 29.19 |
| ATOM | 460 | C   | GLY | 1116 | 89.973 | 39.686 | 57.271 | 1.00 | 27.79 |
| ATOM | 461 | O   | GLY | 1116 | 89.578 | 39.579 | 56.109 | 1.00 | 28.10 |
| ATOM | 462 | N   | SER | 1117 | 89.249 | 40.247 | 58.237 | 1.00 | 25.03 |
| ATOM | 463 | CA  | SER | 1117 | 87.909 | 40.729 | 57.973 | 1.00 | 24.84 |
| ATOM | 464 | CB  | SER | 1117 | 86.904 | 40.042 | 58.899 | 1.00 | 23.52 |
| ATOM | 465 | OG  | SER | 1117 | 86.986 | 40.560 | 60.214 | 1.00 | 21.42 |
| ATOM | 466 | C   | SER | 1117 | 87.800 | 42.226 | 58.161 | 1.00 | 25.97 |
| ATOM | 467 | O   | SER | 1117 | 88.671 | 42.846 | 58.768 | 1.00 | 27.89 |
| ATOM | 468 | N   | ARG | 1118 | 86.742 | 42.796 | 57.591 | 1.00 | 26.62 |
| ATOM | 469 | CA  | ARG | 1118 | 86.416 | 44.208 | 57.719 | 1.00 | 25.45 |
| ATOM | 470 | CB  | ARG | 1118 | 86.940 | 45.048 | 56.545 | 1.00 | 28.49 |
| ATOM | 471 | CG  | ARG | 1118 | 86.095 | 45.116 | 55.292 | 1.00 | 32.87 |
| ATOM | 472 | CD  | ARG | 1118 | 86.240 | 46.504 | 54.632 | 1.00 | 40.52 |
| ATOM | 473 | NE  | ARG | 1118 | 85.263 | 47.482 | 55.135 | 1.00 | 46.91 |
| ATOM | 474 | CZ  | ARG | 1118 | 84.084 | 47.729 | 54.558 | 1.00 | 48.20 |
| ATOM | 475 | NH1 | ARG | 1118 | 83.741 | 47.085 | 53.444 | 1.00 | 49.22 |
| ATOM | 476 | NH2 | ARG | 1118 | 83.217 | 48.567 | 55.114 | 1.00 | 50.55 |
| ATOM | 477 | C   | ARG | 1118 | 84.894 | 44.224 | 57.812 | 1.00 | 24.87 |
| ATOM | 478 | O   | ARG | 1118 | 84.224 | 43.400 | 57.192 | 1.00 | 23.66 |
| ATOM | 479 | N   | SER | 1119 | 84.354 | 45.088 | 58.659 | 1.00 | 24.12 |
| ATOM | 480 | CA  | SER | 1119 | 82.917 | 45.142 | 58.848 | 1.00 | 21.38 |
| ATOM | 481 | CB  | SER | 1119 | 82.566 | 45.698 | 60.221 | 1.00 | 19.53 |
| ATOM | 482 | OG  | SER | 1119 | 82.806 | 44.732 | 61.235 | 1.00 | 18.13 |
| ATOM | 483 | C   | SER | 1119 | 82.134 | 45.881 | 57.789 | 1.00 | 22.88 |
| ATOM | 484 | O   | SER | 1119 | 82.661 | 46.738 | 57.076 | 1.00 | 22.56 |
| ATOM | 485 | N   | LEU | 1120 | 80.872 | 45.486 | 57.682 | 1.00 | 23.25 |
| ATOM | 486 | CA  | LEU | 1120 | 79.915 | 46.057 | 56.758 | 1.00 | 24.37 |
| ATOM | 487 | CB  | LEU | 1120 | 78.950 | 44.979 | 56.290 | 1.00 | 23.76 |
| ATOM | 488 | CG  | LEU | 1120 | 78.911 | 44.542 | 54.840 | 1.00 | 23.49 |
| ATOM | 489 | CD1 | LEU | 1120 | 77.753 | 43.571 | 54.701 | 1.00 | 21.66 |
| ATOM | 490 | CD2 | LEU | 1120 | 78.726 | 45.752 | 53.934 | 1.00 | 22.71 |
| ATOM | 491 | C   | LEU | 1120 | 79.107 | 47.107 | 57.510 | 1.00 | 27.32 |
| ATOM | 492 | O   | LEU | 1120 | 78.891 | 46.994 | 58.725 | 1.00 | 28.09 |
| ATOM | 493 | N   | THR | 1121 | 78.618 | 48.096 | 56.771 | 1.00 | 30.14 |
| ATOM | 494 | CA  | THR | 1121 | 77.821 | 49.176 | 57.334 | 1.00 | 29.30 |
| ATOM | 495 | CB  | THR | 1121 | 78.065 | 50.474 | 56.574 | 1.00 | 29.90 |
| ATOM | 496 | OG1 | THR | 1121 | 79.457 | 50.575 | 56.236 | 1.00 | 32.57 |
| ATOM | 497 | CG2 | THR | 1121 | 77.650 | 51.656 | 57.415 | 1.00 | 28.80 |
| ATOM | 498 | C   | THR | 1121 | 76.361 | 48.835 | 57.150 | 1.00 | 30.05 |
| ATOM | 499 | O   | THR | 1121 | 75.955 | 48.396 | 56.075 | 1.00 | 32.34 |
| ATOM | 500 | N   | PRO | 1122 | 75.546 | 49.021 | 58.190 | 1.00 | 29.89 |
| ATOM | 501 | CD  | PRO | 1122 | 75.910 | 49.352 | 59.571 | 1.00 | 29.08 |
| ATOM | 502 | CA  | PRO | 1122 | 74.118 | 48.717 | 58.088 | 1.00 | 29.25 |
| ATOM | 503 | CB  | PRO | 1122 | 73.637 | 48.907 | 59.517 | 1.00 | 28.58 |
| ATOM | 504 | CG  | PRO | 1122 | 74.856 | 48.613 | 60.323 | 1.00 | 30.38 |

FIGURE 3 (CONT.)

| ATOM | 505 | C | PRO | 1122 | 73.427 | 49.703 | 57.145 | 1.00 | 30.47 |
|------|-----|---|-----|------|--------|--------|--------|------|-------|
| ATOM | 506 | O | PRO | 1122 | 73.874 | 50.839 | 56.986 | 1.00 | 32.91 |
| ATOM | 507 | N | CYS | 1123 | 72.346 | 49.271 | 56.511 | 1.00 | 30.63 |
| ATOM | 508 | CA | CYS | 1123 | 71.621 | 50.136 | 55.596 | 1.00 | 30.60 |
| ATOM | 509 | CB | CYS | 1123 | 70.614 | 49.332 | 54.778 | 1.00 | 29.72 |
| ATOM | 510 | SG | CYS | 1123 | 69.790 | 50.297 | 53.488 | 1.00 | 25.00 |
| ATOM | 511 | C | CYS | 1123 | 70.906 | 51.235 | 56.384 | 1.00 | 32.65 |
| ATOM | 512 | O | CYS | 1123 | 70.541 | 51.047 | 57.546 | 1.00 | 31.99 |
| ATOM | 513 | N | THR | 1124 | 70.744 | 52.393 | 55.755 | 1.00 | 34.65 |
| ATOM | 514 | CA | THR | 1124 | 70.082 | 53.533 | 56.377 | 1.00 | 36.02 |
| ATOM | 515 | CB | THR | 1124 | 71.118 | 54.557 | 56.908 | 1.00 | 36.13 |
| ATOM | 516 | OG1 | THR | 1124 | 71.877 | 55.082 | 55.810 | 1.00 | 36.33 |
| ATOM | 517 | CG2 | THR | 1124 | 72.074 | 53.903 | 57.908 | 1.00 | 34.16 |
| ATOM | 518 | C | THR | 1124 | 69.208 | 54.236 | 55.337 | 1.00 | 37.69 |
| ATOM | 519 | O | THR | 1124 | 68.718 | 55.341 | 55.576 | 1.00 | 40.17 |
| ATOM | 520 | N | CYS | 1125 | 69.040 | 53.609 | 54.174 | 1.00 | 37.56 |
| ATOM | 521 | CA | CYS | 1125 | 68.243 | 54.202 | 53.110 | 1.00 | 35.40 |
| ATOM | 522 | CB | CYS | 1125 | 69.001 | 54.161 | 51.775 | 1.00 | 36.85 |
| ATOM | 523 | SG | CYS | 1125 | 69.270 | 52.512 | 51.083 | 1.00 | 37.80 |
| ATOM | 524 | C | CYS | 1125 | 66.884 | 53.548 | 52.958 | 1.00 | 34.49 |
| ATOM | 525 | O | CYS | 1125 | 66.079 | 53.974 | 52.139 | 1.00 | 36.12 |
| ATOM | 526 | N | GLY | 1126 | 66.637 | 52.496 | 53.725 | 1.00 | 34.32 |
| ATOM | 527 | CA | GLY | 1126 | 65.358 | 51.813 | 53.650 | 1.00 | 33.36 |
| ATOM | 528 | C | GLY | 1126 | 64.953 | 51.332 | 52.271 | 1.00 | 32.12 |
| ATOM | 529 | O | GLY | 1126 | 63.764 | 51.212 | 51.976 | 1.00 | 33.53 |
| ATOM | 530 | N | SER | 1127 | 65.931 | 51.066 | 51.417 | 1.00 | 30.17 |
| ATOM | 531 | CA | SER | 1127 | 65.636 | 50.584 | 50.082 | 1.00 | 30.11 |
| ATOM | 532 | CB | SER | 1127 | 66.886 | 50.595 | 49.220 | 1.00 | 30.14 |
| ATOM | 533 | OG | SER | 1127 | 66.565 | 50.233 | 47.893 | 1.00 | 31.03 |
| ATOM | 534 | C | SER | 1127 | 65.090 | 49.165 | 50.154 | 1.00 | 31.51 |
| ATOM | 535 | O | SER | 1127 | 65.455 | 48.392 | 51.042 | 1.00 | 33.06 |
| ATOM | 536 | N | SER | 1128 | 64.232 | 48.823 | 49.201 | 1.00 | 32.01 |
| ATOM | 537 | CA | SER | 1128 | 63.625 | 47.501 | 49.140 | 1.00 | 32.06 |
| ATOM | 538 | CB | SER | 1128 | 62.125 | 47.633 | 48.916 | 1.00 | 33.84 |
| ATOM | 539 | OG | SER | 1128 | 61.868 | 48.596 | 47.908 | 1.00 | 39.40 |
| ATOM | 540 | C | SER | 1128 | 64.246 | 46.652 | 48.042 | 1.00 | 31.04 |
| ATOM | 541 | O | SER | 1128 | 63.892 | 45.490 | 47.866 | 1.00 | 30.15 |
| ATOM | 542 | N | ASP | 1129 | 65.153 | 47.244 | 47.281 | 1.00 | 31.57 |
| ATOM | 543 | CA | ASP | 1129 | 65.838 | 46.521 | 46.221 | 1.00 | 30.82 |
| ATOM | 544 | CB | ASP | 1129 | 66.170 | 47.478 | 45.071 | 1.00 | 32.94 |
| ATOM | 545 | CG | ASP | 1129 | 64.925 | 48.168 | 44.512 | 1.00 | 37.09 |
| ATOM | 546 | OD1 | ASP | 1129 | 64.087 | 47.488 | 43.876 | 1.00 | 38.85 |
| ATOM | 547 | OD2 | ASP | 1129 | 64.769 | 49.388 | 44.731 | 1.00 | 40.93 |
| ATOM | 548 | C | ASP | 1129 | 67.101 | 45.931 | 46.838 | 1.00 | 28.43 |
| ATOM | 549 | O | ASP | 1129 | 68.110 | 46.617 | 46.966 | 1.00 | 28.53 |
| ATOM | 550 | N | LEU | 1130 | 67.006 | 44.679 | 47.280 | 1.00 | 28.60 |
| ATOM | 551 | CA | LEU | 1130 | 68.114 | 43.965 | 47.922 | 1.00 | 27.20 |
| ATOM | 552 | CB | LEU | 1130 | 67.570 | 43.060 | 49.026 | 1.00 | 25.89 |
| ATOM | 553 | CG | LEU | 1130 | 66.449 | 43.614 | 49.910 | 1.00 | 27.61 |
| ATOM | 554 | CD1 | LEU | 1130 | 66.230 | 42.644 | 51.049 | 1.00 | 30.67 |
| ATOM | 555 | CD2 | LEU | 1130 | 66.781 | 44.991 | 50.455 | 1.00 | 26.86 |

FIGURE 5 (CONT.)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 556 | C | LEU | 1130 | 68.955 | 43.122 | 46.955 | 1.00 | 27.30 |
| ATOM | 557 | O | LEU | 1130 | 68.524 | 42.812 | 45.847 | 1.00 | 29.26 |
| ATOM | 558 | N | TYR | 1131 | 70.155 | 42.740 | 47.386 | 1.00 | 26.38 |
| ATOM | 559 | CA | TYR | 1131 | 71.060 | 41.939 | 46.572 | 1.00 | 24.28 |
| ATOM | 560 | CB | TYR | 1131 | 72.118 | 42.830 | 45.922 | 1.00 | 22.21 |
| ATOM | 561 | CG | TYR | 1131 | 71.528 | 43.904 | 45.044 | 1.00 | 23.22 |
| ATOM | 562 | CD1 | TYR | 1131 | 71.208 | 45.151 | 45.562 | 1.00 | 23.25 |
| ATOM | 563 | CE1 | TYR | 1131 | 70.601 | 46.129 | 44.772 | 1.00 | 25.08 |
| ATOM | 564 | CD2 | TYR | 1131 | 71.234 | 43.654 | 43.707 | 1.00 | 24.48 |
| ATOM | 565 | CE2 | TYR | 1131 | 70.626 | 44.627 | 42.905 | 1.00 | 24.25 |
| ATOM | 566 | CZ | TYR | 1131 | 70.311 | 45.860 | 43.447 | 1.00 | 25.18 |
| ATOM | 567 | OH | TYR | 1131 | 69.697 | 46.824 | 42.673 | 1.00 | 26.26 |
| ATOM | 568 | C | TYR | 1131 | 71.725 | 40.924 | 47.479 | 1.00 | 24.97 |
| ATOM | 569 | O | TYR | 1131 | 72.462 | 41.293 | 48.386 | 1.00 | 27.58 |
| ATOM | 570 | N | LEU | 1132 | 71.431 | 39.649 | 47.259 | 1.00 | 24.30 |
| ATOM | 571 | CA | LEU | 1132 | 71.984 | 38.569 | 48.067 | 1.00 | 24.74 |
| ATOM | 572 | CB | LEU | 1132 | 70.964 | 37.438 | 48.186 | 1.00 | 24.61 |
| ATOM | 573 | CG | LEU | 1132 | 71.334 | 36.245 | 49.064 | 1.00 | 22.52 |
| ATOM | 574 | CD1 | LEU | 1132 | 70.194 | 36.009 | 50.007 | 1.00 | 27.96 |
| ATOM | 575 | CD2 | LEU | 1132 | 71.605 | 35.009 | 48.230 | 1.00 | 23.92 |
| ATOM | 576 | C | LEU | 1132 | 73.276 | 38.023 | 47.489 | 1.00 | 25.14 |
| ATOM | 577 | O | LEU | 1132 | 73.350 | 37.746 | 46.297 | 1.00 | 27.15 |
| ATOM | 578 | N | VAL | 1133 | 74.288 | 37.857 | 48.333 | 1.00 | 25.08 |
| ATOM | 579 | CA | VAL | 1133 | 75.577 | 37.327 | 47.890 | 1.00 | 24.16 |
| ATOM | 580 | CB | VAL | 1133 | 76.757 | 38.156 | 48.445 | 1.00 | 23.60 |
| ATOM | 581 | CG1 | VAL | 1133 | 78.076 | 37.629 | 47.872 | 1.00 | 19.70 |
| ATOM | 582 | CG2 | VAL | 1133 | 76.556 | 39.645 | 48.134 | 1.00 | 18.12 |
| ATOM | 583 | C | VAL | 1133 | 75.719 | 35.890 | 48.377 | 1.00 | 24.92 |
| ATOM | 584 | O | VAL | 1133 | 75.573 | 35.620 | 49.572 | 1.00 | 25.15 |
| ATOM | 585 | N | THR | 1134 | 75.987 | 34.969 | 47.456 | 1.00 | 24.88 |
| ATOM | 586 | CA | THR | 1134 | 76.125 | 33.563 | 47.812 | 1.00 | 25.34 |
| ATOM | 587 | CB | THR | 1134 | 75.611 | 32.638 | 46.677 | 1.00 | 27.21 |
| ATOM | 588 | OG1 | THR | 1134 | 76.498 | 32.698 | 45.550 | 1.00 | 26.50 |
| ATOM | 589 | CG2 | THR | 1134 | 74.204 | 33.054 | 46.236 | 1.00 | 24.71 |
| ATOM | 590 | C | THR | 1134 | 77.566 | 33.205 | 48.150 | 1.00 | 25.73 |
| ATOM | 591 | O | THR | 1134 | 78.476 | 34.010 | 47.944 | 1.00 | 26.83 |
| ATOM | 592 | N | ARG | 1135 | 77.776 | 31.981 | 48.630 | 1.00 | 25.40 |
| ATOM | 593 | CA | ARG | 1135 | 79.112 | 31.504 | 48.991 | 1.00 | 23.76 |
| ATOM | 594 | CB | ARG | 1135 | 79.027 | 30.150 | 49.689 | 1.00 | 22.71 |
| ATOM | 595 | CG | ARG | 1135 | 78.413 | 29.062 | 48.835 | 1.00 | 25.45 |
| ATOM | 596 | CD | ARG | 1135 | 78.383 | 27.742 | 49.566 | 1.00 | 26.50 |
| ATOM | 597 | NE | ARG | 1135 | 79.722 | 27.265 | 49.897 | 1.00 | 27.92 |
| ATOM | 598 | CZ | ARG | 1135 | 80.174 | 27.097 | 51.135 | 1.00 | 27.79 |
| ATOM | 599 | NH1 | ARG | 1135 | 79.405 | 27.366 | 52.180 | 1.00 | 28.04 |
| ATOM | 600 | NH2 | ARG | 1135 | 81.404 | 26.652 | 51.327 | 1.00 | 30.59 |
| ATOM | 601 | C | ARG | 1135 | 80.038 | 31.382 | 47.792 | 1.00 | 24.58 |
| ATOM | 602 | O | ARG | 1135 | 81.219 | 31.091 | 47.950 | 1.00 | 25.10 |
| ATOM | 603 | N | HIS | 1136 | 79.496 | 31.546 | 46.589 | 1.00 | 25.35 |
| ATOM | 604 | CA | HIS | 1136 | 80.303 | 31.451 | 45.378 | 1.00 | 26.27 |
| ATOM | 605 | CB | HIS | 1136 | 79.618 | 30.551 | 44.348 | 1.00 | 26.38 |
| ATOM | 606 | CG | HIS | 1136 | 79.283 | 29.194 | 44.872 | 1.00 | 27.82 |

15/60

FIGURE 3 (CONT.)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 607 | CD2 | HIS | 1136 | 78.091 | 28.629 | 45.174 | 1.00 | 28.51 |
| ATOM | 608 | ND1 | HIS | 1136 | 80.242 | 28.264 | 45.213 | 1.00 | 29.89 |
| ATOM | 609 | CE1 | HIS | 1136 | 79.657 | 27.188 | 45.710 | 1.00 | 29.44 |
| ATOM | 610 | NE2 | HIS | 1136 | 78.353 | 27.387 | 45.697 | 1.00 | 31.77 |
| ATOM | 611 | C | HIS | 1136 | 80.540 | 32.834 | 44.794 | 1.00 | 26.66 |
| ATOM | 612 | O | HIS | 1136 | 81.064 | 32.966 | 43.686 | 1.00 | 27.04 |
| ATOM | 613 | N | ALA | 1137 | 80.126 | 33.850 | 45.552 | 1.00 | 26.65 |
| ATOM | 614 | CA | ALA | 1137 | 80.265 | 35.253 | 45.179 | 1.00 | 25.32 |
| ATOM | 615 | CB | ALA | 1137 | 81.675 | 35.532 | 44.664 | 1.00 | 26.21 |
| ATOM | 616 | C | ALA | 1137 | 79.219 | 35.743 | 44.177 | 1.00 | 25.87 |
| ATOM | 617 | O | ALA | 1137 | 79.280 | 36.890 | 43.724 | 1.00 | 24.80 |
| ATOM | 618 | N | ASP | 1138 | 78.256 | 34.887 | 43.837 | 1.00 | 24.81 |
| ATOM | 619 | CA | ASP | 1138 | 77.203 | 35.277 | 42.903 | 1.00 | 23.77 |
| ATOM | 620 | CB | ASP | 1138 | 76.301 | 34.091 | 42.536 | 1.00 | 26.17 |
| ATOM | 621 | CG | ASP | 1138 | 77.038 | 32.962 | 41.827 | 1.00 | 27.49 |
| ATOM | 622 | OD1 | ASP | 1138 | 77.712 | 33.214 | 40.807 | 1.00 | 27.61 |
| ATOM | 623 | OD2 | ASP | 1138 | 76.891 | 31.801 | 42.268 | 1.00 | 28.37 |
| ATOM | 624 | C | ASP | 1138 | 76.344 | 36.301 | 43.629 | 1.00 | 22.53 |
| ATOM | 625 | O | ASP | 1138 | 76.282 | 36.302 | 44.856 | 1.00 | 23.66 |
| ATOM | 626 | N | VAL | 1139 | 75.699 | 37.180 | 42.881 | 1.00 | 21.63 |
| ATOM | 627 | CA | VAL | 1139 | 74.828 | 38.178 | 43.477 | 1.00 | 22.35 |
| ATOM | 628 | CB | VAL | 1139 | 75.287 | 39.627 | 43.161 | 1.00 | 20.65 |
| ATOM | 629 | CG1 | VAL | 1139 | 74.385 | 40.625 | 43.854 | 1.00 | 17.61 |
| ATOM | 630 | CG2 | VAL | 1139 | 76.736 | 39.841 | 43.607 | 1.00 | 16.25 |
| ATOM | 631 | C | VAL | 1139 | 73.438 | 37.908 | 42.915 | 1.00 | 24.89 |
| ATOM | 632 | O | VAL | 1139 | 73.270 | 37.696 | 41.706 | 1.00 | 27.94 |
| ATOM | 633 | N | ILE | 1140 | 72.447 | 37.895 | 43.796 | 1.00 | 24.15 |
| ATOM | 634 | CA | ILE | 1140 | 71.071 | 37.606 | 43.425 | 1.00 | 21.78 |
| ATOM | 635 | CB | ILE | 1140 | 70.588 | 36.338 | 44.156 | 1.00 | 19.13 |
| ATOM | 636 | CG2 | ILE | 1140 | 69.104 | 36.166 | 43.999 | 1.00 | 19.57 |
| ATOM | 637 | CG1 | ILE | 1140 | 71.329 | 35.104 | 43.647 | 1.00 | 17.97 |
| ATOM | 638 | CD1 | ILE | 1140 | 71.069 | 33.877 | 44.498 | 1.00 | 16.36 |
| ATOM | 639 | C | ILE | 1140 | 70.149 | 38.748 | 43.816 | 1.00 | 22.53 |
| ATOM | 640 | O | ILE | 1140 | 69.979 | 39.038 | 44.995 | 1.00 | 23.66 |
| ATOM | 641 | N | PRO | 1141 | 69.546 | 39.422 | 42.832 | 1.00 | 23.25 |
| ATOM | 642 | CD | PRO | 1141 | 69.768 | 39.320 | 41.383 | 1.00 | 22.90 |
| ATOM | 643 | CA | PRO | 1141 | 68.638 | 40.530 | 43.144 | 1.00 | 23.97 |
| ATOM | 644 | CB | PRO | 1141 | 68.328 | 41.111 | 41.770 | 1.00 | 24.50 |
| ATOM | 645 | CG | PRO | 1141 | 69.549 | 40.730 | 40.952 | 1.00 | 24.13 |
| ATOM | 646 | C | PRO | 1141 | 67.372 | 40.003 | 43.835 | 1.00 | 26.14 |
| ATOM | 647 | O | PRO | 1141 | 66.692 | 39.095 | 43.341 | 1.00 | 27.20 |
| ATOM | 648 | N | VAL | 1142 | 67.085 | 40.556 | 44.999 | 1.00 | 26.19 |
| ATOM | 649 | CA | VAL | 1142 | 65.936 | 40.161 | 45.788 | 1.00 | 27.02 |
| ATOM | 650 | CB | VAL | 1142 | 66.406 | 39.499 | 47.096 | 1.00 | 25.62 |
| ATOM | 651 | CG1 | VAL | 1142 | 65.263 | 39.348 | 48.074 | 1.00 | 24.17 |
| ATOM | 652 | CG2 | VAL | 1142 | 67.036 | 38.155 | 46.787 | 1.00 | 24.42 |
| ATOM | 653 | C | VAL | 1142 | 65.136 | 41.422 | 46.087 | 1.00 | 29.57 |
| ATOM | 654 | O | VAL | 1142 | 65.703 | 42.462 | 46.413 | 1.00 | 30.26 |
| ATOM | 655 | N | ARG | 1143 | 63.827 | 41.358 | 45.896 | 1.00 | 31.86 |
| ATOM | 656 | CA | ARG | 1143 | 62.989 | 42.512 | 46.166 | 1.00 | 35.28 |
| ATOM | 657 | CB | ARG | 1143 | 61.964 | 42.715 | 45.053 | 1.00 | 38.62 |

FIGURE 3 (CONT.)

| | | | | | | | | | |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 658 | CG | ARG | 1143 | 61.555 | 44.152 | 44.880 | 1.00 | 40.15 |
| ATOM | 659 | CD | ARG | 1143 | 60.377 | 44.489 | 45.748 | 1.00 | 44.51 |
| ATOM | 660 | NE | ARG | 1143 | 60.308 | 45.904 | 46.106 | 1.00 | 51.14 |
| ATOM | 661 | CZ | ARG | 1143 | 60.485 | 46.926 | 45.269 | 1.00 | 55.15 |
| ATOM | 662 | NH1 | ARG | 1143 | 60.759 | 46.731 | 43.983 | 1.00 | 57.46 |
| ATOM | 663 | NH2 | ARG | 1143 | 60.355 | 48.166 | 45.723 | 1.00 | 57.00 |
| ATOM | 664 | C | ARG | 1143 | 62.316 | 42.243 | 47.497 | 1.00 | 36.53 |
| ATOM | 665 | O | ARG | 1143 | 61.696 | 41.197 | 47.695 | 1.00 | 39.63 |
| ATOM | 666 | N | ARG | 1144 | 62.474 | 43.171 | 48.425 | 1.00 | 36.31 |
| ATOM | 667 | CA | ARG | 1144 | 61.917 | 43.010 | 49.750 | 1.00 | 36.40 |
| ATOM | 668 | CB | ARG | 1144 | 62.448 | 44.090 | 50.673 | 1.00 | 35.36 |
| ATOM | 669 | CG | ARG | 1144 | 62.311 | 43.749 | 52.125 | 1.00 | 35.23 |
| ATOM | 670 | CD | ARG | 1144 | 62.817 | 44.882 | 52.953 | 1.00 | 36.19 |
| ATOM | 671 | NE | ARG | 1144 | 62.992 | 44.497 | 54.346 | 1.00 | 39.02 |
| ATOM | 672 | CZ | ARG | 1144 | 63.660 | 45.233 | 55.223 | 1.00 | 40.02 |
| ATOM | 673 | NH1 | ARG | 1144 | 63.786 | 44.834 | 56.481 | 1.00 | 38.46 |
| ATOM | 674 | NH2 | ARG | 1144 | 64.205 | 46.377 | 54.831 | 1.00 | 42.18 |
| ATOM | 675 | C | ARG | 1144 | 60.405 | 43.041 | 49.742 | 1.00 | 38.06 |
| ATOM | 676 | O | ARG | 1144 | 59.784 | 43.800 | 48.995 | 1.00 | 37.65 |
| ATOM | 677 | N | ARG | 1145 | 59.820 | 42.193 | 50.575 | 1.00 | 40.25 |
| ATOM | 678 | CA | ARG | 1145 | 58.377 | 42.107 | 50.689 | 1.00 | 41.89 |
| ATOM | 679 | CB | ARG | 1145 | 57.897 | 40.717 | 50.278 | 1.00 | 40.89 |
| ATOM | 680 | CG | ARG | 1145 | 58.127 | 40.425 | 48.805 | 1.00 | 40.67 |
| ATOM | 681 | CD | ARG | 1145 | 57.432 | 41.454 | 47.960 | 1.00 | 40.17 |
| ATOM | 682 | NE | ARG | 1145 | 57.599 | 41.235 | 46.530 | 1.00 | 41.36 |
| ATOM | 683 | CZ | ARG | 1145 | 57.295 | 42.146 | 45.612 | 1.00 | 45.08 |
| ATOM | 684 | NH1 | ARG | 1145 | 56.814 | 43.332 | 45.982 | 1.00 | 47.79 |
| ATOM | 685 | NH2 | ARG | 1145 | 57.465 | 41.878 | 44.324 | 1.00 | 45.53 |
| ATOM | 686 | C | ARG | 1145 | 57.903 | 42.458 | 52.090 | 1.00 | 42.89 |
| ATOM | 687 | O | ARG | 1145 | 56.720 | 42.725 | 52.295 | 1.00 | 44.14 |
| ATOM | 688 | N | GLY | 1146 | 58.832 | 42.493 | 53.043 | 1.00 | 43.96 |
| ATOM | 689 | CA | GLY | 1146 | 58.483 | 42.832 | 54.412 | 1.00 | 44.02 |
| ATOM | 690 | C | GLY | 1146 | 59.699 | 42.813 | 55.312 | 1.00 | 43.54 |
| ATOM | 691 | O | GLY | 1146 | 60.795 | 42.495 | 54.847 | 1.00 | 44.52 |
| ATOM | 692 | N | ASP | 1147 | 59.499 | 43.110 | 56.595 | 1.00 | 42.52 |
| ATOM | 693 | CA | ASP | 1147 | 60.570 | 43.134 | 57.596 | 1.00 | 40.57 |
| ATOM | 694 | CB | ASP | 1147 | 59.987 | 43.005 | 59.013 | 1.00 | 45.28 |
| ATOM | 695 | CG | ASP | 1147 | 59.051 | 44.151 | 59.382 | 1.00 | 51.16 |
| ATOM | 696 | OD1 | ASP | 1147 | 58.092 | 43.897 | 60.151 | 1.00 | 53.15 |
| ATOM | 697 | OD2 | ASP | 1147 | 59.271 | 45.296 | 58.916 | 1.00 | 54.39 |
| ATOM | 698 | C | ASP | 1147 | 61.665 | 42.080 | 57.424 | 1.00 | 37.05 |
| ATOM | 699 | O | ASP | 1147 | 62.845 | 42.387 | 57.552 | 1.00 | 37.14 |
| ATOM | 700 | N | SER | 1148 | 61.283 | 40.840 | 57.150 | 1.00 | 32.32 |
| ATOM | 701 | CA | SER | 1148 | 62.278 | 39.794 | 56.996 | 1.00 | 30.82 |
| ATOM | 702 | CB | SER | 1148 | 62.436 | 39.055 | 58.321 | 1.00 | 32.46 |
| ATOM | 703 | OG | SER | 1148 | 61.246 | 38.376 | 58.667 | 1.00 | 35.71 |
| ATOM | 704 | C | SER | 1148 | 62.013 | 38.801 | 55.866 | 1.00 | 28.99 |
| ATOM | 705 | O | SER | 1148 | 62.313 | 37.619 | 56.003 | 1.00 | 26.58 |
| ATOM | 706 | N | ARG | 1149 | 61.504 | 39.288 | 54.736 | 1.00 | 29.34 |
| ATOM | 707 | CA | ARG | 1149 | 61.211 | 38.426 | 53.589 | 1.00 | 30.00 |
| ATOM | 708 | CB | ARG | 1149 | 59.760 | 37.914 | 53.663 | 1.00 | 33.43 |

FIGURE 3 (CONT.)

| ATOM | 709 | CG | ARG | 1149 | 59.363 | 36.826 | 52.655 | 1.00 | 36.36 |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 710 | CD | ARG | 1149 | 58.733 | 37.418 | 51.389 | 1.00 | 42.94 |
| ATOM | 711 | NE | ARG | 1149 | 57.958 | 36.444 | 50.610 | 1.00 | 46.67 |
| ATOM | 712 | CZ | ARG | 1149 | 57.764 | 36.514 | 49.291 | 1.00 | 46.83 |
| ATOM | 713 | NH1 | ARG | 1149 | 58.288 | 37.506 | 48.594 | 1.00 | 45.95 |
| ATOM | 714 | NH2 | ARG | 1149 | 57.021 | 35.603 | 48.668 | 1.00 | 47.58 |
| ATOM | 715 | C | ARG | 1149 | 61.442 | 39.191 | 52.290 | 1.00 | 28.92 |
| ATOM | 716 | O | ARG | 1149 | 61.181 | 40.401 | 52.206 | 1.00 | 27.96 |
| ATOM | 717 | N | GLY | 1150 | 61.921 | 38.471 | 51.282 | 1.00 | 27.08 |
| ATOM | 718 | CA | GLY | 1150 | 62.190 | 39.065 | 49.986 | 1.00 | 25.77 |
| ATOM | 719 | C | GLY | 1150 | 61.983 | 38.029 | 48.900 | 1.00 | 25.52 |
| ATOM | 720 | O | GLY | 1150 | 62.093 | 36.831 | 49.147 | 1.00 | 24.50 |
| ATOM | 721 | N | SER | 1151 | 61.672 | 38.479 | 47.694 | 1.00 | 25.63 |
| ATOM | 722 | CA | SER | 1151 | 61.441 | 37.572 | 46.583 | 1.00 | 27.27 |
| ATOM | 723 | CB | SER | 1151 | 60.076 | 37.859 | 45.960 | 1.00 | 29.08 |
| ATOM | 724 | OG | SER | 1151 | 59.833 | 39.257 | 45.883 | 1.00 | 29.83 |
| ATOM | 725 | C | SER | 1151 | 62.528 | 37.718 | 45.533 | 1.00 | 27.69 |
| ATOM | 726 | O | SER | 1151 | 62.885 | 38.837 | 45.150 | 1.00 | 28.46 |
| ATOM | 727 | N | LEU | 1152 | 63.093 | 36.592 | 45.109 | 1.00 | 26.82 |
| ATOM | 728 | CA | LEU | 1152 | 64.129 | 36.609 | 44.089 | 1.00 | 27.90 |
| ATOM | 729 | CB | LEU | 1152 | 64.658 | 35.202 | 43.828 | 1.00 | 24.63 |
| ATOM | 730 | CG | LEU | 1152 | 65.784 | 34.643 | 44.686 | 1.00 | 23.94 |
| ATOM | 731 | CD1 | LEU | 1152 | 65.377 | 34.577 | 46.139 | 1.00 | 22.37 |
| ATOM | 732 | CD2 | LEU | 1152 | 66.145 | 33.273 | 44.155 | 1.00 | 19.80 |
| ATOM | 733 | C | LEU | 1152 | 63.501 | 37.127 | 42.811 | 1.00 | 29.83 |
| ATOM | 734 | O | LEU | 1152 | 62.394 | 36.722 | 42.463 | 1.00 | 33.35 |
| ATOM | 735 | N | LEU | 1153 | 64.199 | 38.009 | 42.107 | 1.00 | 30.33 |
| ATOM | 736 | CA | LEU | 1153 | 63.676 | 38.538 | 40.858 | 1.00 | 29.78 |
| ATOM | 737 | CB | LEU | 1153 | 64.521 | 39.716 | 40.379 | 1.00 | 26.59 |
| ATOM | 738 | CG | LEU | 1153 | 64.020 | 41.065 | 40.896 | 1.00 | 25.76 |
| ATOM | 739 | CD1 | LEU | 1153 | 63.897 | 41.039 | 42.394 | 1.00 | 24.26 |
| ATOM | 740 | CD2 | LEU | 1153 | 64.940 | 42.176 | 40.444 | 1.00 | 26.30 |
| ATOM | 741 | C | LEU | 1153 | 63.643 | 37.433 | 39.808 | 1.00 | 31.23 |
| ATOM | 742 | O | LEU | 1153 | 62.853 | 37.474 | 38.869 | 1.00 | 33.74 |
| ATOM | 743 | N | SER | 1154 | 64.503 | 36.440 | 39.987 | 1.00 | 32.78 |
| ATOM | 744 | CA | SER | 1154 | 64.596 | 35.309 | 39.081 | 1.00 | 34.85 |
| ATOM | 745 | CB | SER | 1154 | 65.780 | 35.481 | 38.132 | 1.00 | 36.29 |
| ATOM | 746 | OG | SER | 1154 | 65.855 | 36.805 | 37.636 | 1.00 | 43.91 |
| ATOM | 747 | C | SER | 1154 | 64.846 | 34.107 | 39.961 | 1.00 | 35.31 |
| ATOM | 748 | O | SER | 1154 | 65.943 | 33.949 | 40.505 | 1.00 | 37.17 |
| ATOM | 749 | N | PRO | 1155 | 63.807 | 33.291 | 40.190 | 1.00 | 35.71 |
| ATOM | 750 | CD | PRO | 1155 | 62.401 | 33.474 | 39.780 | 1.00 | 36.01 |
| ATOM | 751 | CA | PRO | 1155 | 63.949 | 32.101 | 41.031 | 1.00 | 34.86 |
| ATOM | 752 | CB | PRO | 1155 | 62.599 | 31.419 | 40.871 | 1.00 | 35.84 |
| ATOM | 753 | CG | PRO | 1155 | 61.670 | 32.598 | 40.777 | 1.00 | 36.09 |
| ATOM | 754 | C | PRO | 1155 | 65.101 | 31.245 | 40.540 | 1.00 | 33.69 |
| ATOM | 755 | O | PRO | 1155 | 65.426 | 31.254 | 39.352 | 1.00 | 33.22 |
| ATOM | 756 | N | ARG | 1156 | 65.726 | 30.525 | 41.459 | 1.00 | 33.17 |
| ATOM | 757 | CA | ARG | 1156 | 66.873 | 29.700 | 41.124 | 1.00 | 35.02 |
| ATOM | 758 | CB | ARG | 1156 | 68.173 | 30.405 | 41.566 | 1.00 | 37.90 |
| ATOM | 759 | CG | ARG | 1156 | 68.856 | 31.265 | 40.505 | 1.00 | 40.72 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 760 | CD | ARG | 1156 | 68.739 | 32.740 | 40.813 | 1.00 | 43.82 |
| ATOM | 761 | NE | ARG | 1156 | 69.536 | 33.543 | 39.886 | 1.00 | 49.55 |
| ATOM | 762 | CZ | ARG | 1156 | 69.696 | 34.864 | 39.972 | 1.00 | 51.56 |
| ATOM | 763 | NH1 | ARG | 1156 | 69.117 | 35.551 | 40.943 | 1.00 | 52.24 |
| ATOM | 764 | NH2 | ARG | 1156 | 70.452 | 35.502 | 39.089 | 1.00 | 53.76 |
| ATOM | 765 | C | ARG | 1156 | 66.799 | 28.348 | 41.804 | 1.00 | 34.39 |
| ATOM | 766 | O | ARG | 1156 | 66.115 | 28.193 | 42.811 | 1.00 | 35.64 |
| ATOM | 767 | N | PRO | 1157 | 67.501 | 27.344 | 41.258 | 1.00 | 34.78 |
| ATOM | 768 | CD | PRO | 1157 | 68.361 | 27.376 | 40.063 | 1.00 | 36.56 |
| ATOM | 769 | CA | PRO | 1157 | 67.495 | 26.008 | 41.859 | 1.00 | 35.76 |
| ATOM | 770 | CB | PRO | 1157 | 68.577 | 25.277 | 41.066 | 1.00 | 35.08 |
| ATOM | 771 | CG | PRO | 1157 | 68.488 | 25.916 | 39.721 | 1.00 | 36.87 |
| ATOM | 772 | C | PRO | 1157 | 67.930 | 26.189 | 43.305 | 1.00 | 36.38 |
| ATOM | 773 | O | PRO | 1157 | 68.824 | 26.993 | 43.579 | 1.00 | 38.01 |
| ATOM | 774 | N | ILE | 1158 | 67.317 | 25.456 | 44.226 | 1.00 | 35.10 |
| ATOM | 775 | CA | ILE | 1158 | 67.675 | 25.599 | 45.629 | 1.00 | 33.87 |
| ATOM | 776 | CB | ILE | 1158 | 66.917 | 24.586 | 46.526 | 1.00 | 33.81 |
| ATOM | 777 | CG2 | ILE | 1158 | 67.042 | 23.174 | 45.973 | 1.00 | 34.22 |
| ATOM | 778 | CG1 | ILE | 1158 | 67.418 | 24.690 | 47.972 | 1.00 | 36.64 |
| ATOM | 779 | CD1 | ILE | 1158 | 66.985 | 23.541 | 48.876 | 1.00 | 38.94 |
| ATOM | 780 | C | ILE | 1158 | 69.185 | 25.486 | 45.834 | 1.00 | 32.49 |
| ATOM | 781 | O | ILE | 1158 | 69.765 | 26.236 | 46.610 | 1.00 | 32.56 |
| ATOM | 782 | N | SER | 1159 | 69.830 | 24.609 | 45.075 | 1.00 | 32.75 |
| ATOM | 783 | CA | SER | 1159 | 71.271 | 24.418 | 45.203 | 1.00 | 33.76 |
| ATOM | 784 | CB | SER | 1159 | 71.769 | 23.392 | 44.188 | 1.00 | 33.12 |
| ATOM | 785 | OG | SER | 1159 | 71.450 | 23.816 | 42.875 | 1.00 | 38.29 |
| ATOM | 786 | C | SER | 1159 | 72.035 | 25.722 | 45.028 | 1.00 | 32.08 |
| ATOM | 787 | O | SER | 1159 | 73.003 | 25.971 | 45.737 | 1.00 | 31.63 |
| ATOM | 788 | N | TYR | 1160 | 71.591 | 26.554 | 44.092 | 1.00 | 29.65 |
| ATOM | 789 | CA | TYR | 1160 | 72.255 | 27.822 | 43.835 | 1.00 | 27.91 |
| ATOM | 790 | CB | TYR | 1160 | 71.482 | 28.628 | 42.798 | 1.00 | 23.87 |
| ATOM | 791 | CG | TYR | 1160 | 72.293 | 29.740 | 42.158 | 1.00 | 22.81 |
| ATOM | 792 | CD1 | TYR | 1160 | 73.402 | 29.455 | 41.368 | 1.00 | 22.72 |
| ATOM | 793 | CE1 | TYR | 1160 | 74.132 | 30.476 | 40.755 | 1.00 | 23.32 |
| ATOM | 794 | CD2 | TYR | 1160 | 71.934 | 31.078 | 42.319 | 1.00 | 23.14 |
| ATOM | 795 | CE2 | TYR | 1160 | 72.656 | 32.104 | 41.704 | 1.00 | 21.74 |
| ATOM | 796 | CZ | TYR | 1160 | 73.749 | 31.793 | 40.928 | 1.00 | 22.91 |
| ATOM | 797 | OH | TYR | 1160 | 74.454 | 32.793 | 40.307 | 1.00 | 24.05 |
| ATOM | 798 | C | TYR | 1160 | 72.413 | 28.638 | 45.118 | 1.00 | 29.71 |
| ATOM | 799 | O | TYR | 1160 | 73.381 | 29.400 | 45.258 | 1.00 | 32.87 |
| ATOM | 800 | N | LEU | 1161 | 71.479 | 28.469 | 46.054 | 1.00 | 27.50 |
| ATOM | 801 | CA | LEU | 1161 | 71.522 | 29.192 | 47.320 | 1.00 | 26.61 |
| ATOM | 802 | CB | LEU | 1161 | 70.140 | 29.752 | 47.670 | 1.00 | 26.28 |
| ATOM | 803 | CG | LEU | 1161 | 69.679 | 31.031 | 46.958 | 1.00 | 28.68 |
| ATOM | 804 | CD1 | LEU | 1161 | 69.484 | 30.775 | 45.469 | 1.00 | 29.40 |
| ATOM | 805 | CD2 | LEU | 1161 | 68.392 | 31.543 | 47.585 | 1.00 | 26.34 |
| ATOM | 806 | C | LEU | 1161 | 72.054 | 28.374 | 48.495 | 1.00 | 26.66 |
| ATOM | 807 | O | LEU | 1161 | 72.247 | 28.905 | 49.588 | 1.00 | 28.59 |
| ATOM | 808 | N | ALA | 1162 | 72.297 | 27.089 | 48.275 | 1.00 | 26.43 |
| ATOM | 809 | CA | ALA | 1162 | 72.790 | 26.213 | 49.330 | 1.00 | 26.08 |
| ATOM | 810 | CB | ALA | 1162 | 72.854 | 24.773 | 48.833 | 1.00 | 27.54 |

FIGURE 3 (CONT.)

| ATOM | 811 | C | ALA | 1162 | 74.148 | 26.638 | 49.878 | 1.00 | 26.55 |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 812 | O | ALA | 1162 | 75.035 | 27.049 | 49.132 | 1.00 | 25.22 |
| ATOM | 813 | N | GLY | 1163 | 74.294 | 26.505 | 51.193 | 1.00 | 26.94 |
| ATOM | 814 | CA | GLY | 1163 | 75.526 | 26.857 | 51.869 | 1.00 | 24.56 |
| ATOM | 815 | C | GLY | 1163 | 75.724 | 28.351 | 52.043 | 1.00 | 25.00 |
| ATOM | 816 | O | GLY | 1163 | 76.767 | 28.771 | 52.529 | 1.00 | 26.71 |
| ATOM | 817 | N | SER | 1164 | 74.718 | 29.151 | 51.704 | 1.00 | 23.80 |
| ATOM | 818 | CA | SER | 1164 | 74.839 | 30.597 | 51.805 | 1.00 | 23.26 |
| ATOM | 819 | CB | SER | 1164 | 74.376 | 31.267 | 50.503 | 1.00 | 23.11 |
| ATOM | 820 | OG | SER | 1164 | 75.068 | 30.759 | 49.372 | 1.00 | 25.78 |
| ATOM | 821 | C | SER | 1164 | 74.115 | 31.243 | 52.968 | 1.00 | 23.96 |
| ATOM | 822 | O | SER | 1164 | 74.153 | 32.466 | 53.102 | 1.00 | 26.14 |
| ATOM | 823 | N | SER | 1165 | 73.412 | 30.474 | 53.789 | 1.00 | 25.28 |
| ATOM | 824 | CA | SER | 1165 | 72.719 | 31.113 | 54.905 | 1.00 | 26.92 |
| ATOM | 825 | CB | SER | 1165 | 71.788 | 30.142 | 55.647 | 1.00 | 29.04 |
| ATOM | 826 | OG | SER | 1165 | 72.468 | 28.977 | 56.096 | 1.00 | 35.95 |
| ATOM | 827 | C | SER | 1165 | 73.790 | 31.695 | 55.820 | 1.00 | 24.96 |
| ATOM | 828 | O | SER | 1165 | 74.785 | 31.036 | 56.126 | 1.00 | 25.60 |
| ATOM | 829 | N | GLY | 1166 | 73.610 | 32.951 | 56.193 | 1.00 | 23.93 |
| ATOM | 830 | CA | GLY | 1166 | 74.582 | 33.630 | 57.026 | 1.00 | 22.49 |
| ATOM | 831 | C | GLY | 1166 | 75.176 | 34.762 | 56.207 | 1.00 | 22.45 |
| ATOM | 832 | O | GLY | 1166 | 75.788 | 35.677 | 56.752 | 1.00 | 20.96 |
| ATOM | 833 | N | GLY | 1167 | 74.965 | 34.692 | 54.892 | 1.00 | 22.45 |
| ATOM | 834 | CA | GLY | 1167 | 75.452 | 35.697 | 53.964 | 1.00 | 22.73 |
| ATOM | 835 | C | GLY | 1167 | 74.687 | 37.003 | 54.055 | 1.00 | 21.55 |
| ATOM | 836 | O | GLY | 1167 | 73.648 | 37.067 | 54.712 | 1.00 | 21.50 |
| ATOM | 837 | N | PRO | 1168 | 75.161 | 38.061 | 53.384 | 1.00 | 20.49 |
| ATOM | 838 | CD | PRO | 1168 | 76.450 | 38.180 | 52.673 | 1.00 | 18.54 |
| ATOM | 839 | CA | PRO | 1168 | 74.478 | 39.354 | 53.439 | 1.00 | 20.96 |
| ATOM | 840 | CB | PRO | 1168 | 75.638 | 40.333 | 53.300 | 1.00 | 17.41 |
| ATOM | 841 | CG | PRO | 1168 | 76.463 | 39.663 | 52.235 | 1.00 | 16.92 |
| ATOM | 842 | C | PRO | 1168 | 73.424 | 39.644 | 52.368 | 1.00 | 21.87 |
| ATOM | 843 | O | PRO | 1168 | 73.480 | 39.127 | 51.251 | 1.00 | 23.31 |
| ATOM | 844 | N | LEU | 1169 | 72.472 | 40.496 | 52.731 | 1.00 | 20.95 |
| ATOM | 845 | CA | LEU | 1169 | 71.441 | 40.950 | 51.818 | 1.00 | 20.67 |
| ATOM | 846 | CB | LEU | 1169 | 70.045 | 40.673 | 52.381 | 1.00 | 22.16 |
| ATOM | 847 | CG | LEU | 1169 | 69.367 | 39.460 | 51.733 | 1.00 | 23.29 |
| ATOM | 848 | CD1 | LEU | 1169 | 68.426 | 38.826 | 52.686 | 1.00 | 25.16 |
| ATOM | 849 | CD2 | LEU | 1169 | 68.652 | 39.858 | 50.459 | 1.00 | 24.84 |
| ATOM | 850 | C | LEU | 1169 | 71.751 | 42.432 | 51.781 | 1.00 | 20.26 |
| ATOM | 851 | O | LEU | 1169 | 71.537 | 43.142 | 52.761 | 1.00 | 20.99 |
| ATOM | 852 | N | LEU | 1170 | 72.369 | 42.855 | 50.686 | 1.00 | 20.65 |
| ATOM | 853 | CA | LEU | 1170 | 72.812 | 44.230 | 50.477 | 1.00 | 20.86 |
| ATOM | 854 | CB | LEU | 1170 | 74.097 | 44.217 | 49.647 | 1.00 | 18.73 |
| ATOM | 855 | CG | LEU | 1170 | 75.246 | 43.277 | 50.028 | 1.00 | 19.61 |
| ATOM | 856 | CD1 | LEU | 1170 | 76.349 | 43.392 | 48.987 | 1.00 | 17.63 |
| ATOM | 857 | CD2 | LEU | 1170 | 75.772 | 43.597 | 51.419 | 1.00 | 15.34 |
| ATOM | 858 | C | LEU | 1170 | 71.820 | 45.149 | 49.774 | 1.00 | 22.02 |
| ATOM | 859 | O | LEU | 1170 | 71.111 | 44.729 | 48.868 | 1.00 | 25.14 |
| ATOM | 860 | N | CYS | 1171 | 71.801 | 46.414 | 50.171 | 1.00 | 22.01 |
| ATOM | 861 | CA | CYS | 1171 | 70.930 | 47.395 | 49.543 | 1.00 | 22.45 |

20/60

FIGURE 3 (CONT.)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 862 | CB | CYS | 1171 | 70.628 | 48.524 | 50.531 | 1.00 | 22.30 |
| ATOM | 863 | SG | CYS | 1171 | 71.982 | 49.681 | 50.780 | 1.00 | 26.39 |
| ATOM | 864 | C | CYS | 1171 | 71.712 | 47.929 | 48.332 | 1.00 | 23.53 |
| ATOM | 865 | O | CYS | 1171 | 72.858 | 47.527 | 48.110 | 1.00 | 22.06 |
| ATOM | 866 | N | PRO | 1172 | 71.124 | 48.850 | 47.542 | 1.00 | 25.28 |
| ATOM | 867 | CD | PRO | 1172 | 69.721 | 49.317 | 47.553 | 1.00 | 23.57 |
| ATOM | 868 | CA | PRO | 1172 | 71.830 | 49.396 | 46.371 | 1.00 | 23.81 |
| ATOM | 869 | CB | PRO | 1172 | 70.831 | 50.418 | 45.834 | 1.00 | 22.44 |
| ATOM | 870 | CG | PRO | 1172 | 69.517 | 49.769 | 46.131 | 1.00 | 21.24 |
| ATOM | 871 | C | PRO | 1172 | 73.188 | 50.054 | 46.661 | 1.00 | 24.42 |
| ATOM | 872 | O | PRO | 1172 | 73.981 | 50.288 | 45.746 | 1.00 | 25.44 |
| ATOM | 873 | N | ALA | 1173 | 73.446 | 50.366 | 47.927 | 1.00 | 23.25 |
| ATOM | 874 | CA | ALA | 1173 | 74.691 | 51.010 | 48.333 | 1.00 | 22.05 |
| ATOM | 875 | CB | ALA | 1173 | 74.381 | 52.102 | 49.356 | 1.00 | 19.70 |
| ATOM | 876 | C | ALA | 1173 | 75.731 | 50.033 | 48.903 | 1.00 | 21.83 |
| ATOM | 877 | O | ALA | 1173 | 76.794 | 50.449 | 49.365 | 1.00 | 21.56 |
| ATOM | 878 | N | GLY | 1174 | 75.402 | 48.745 | 48.911 | 1.00 | 20.69 |
| ATOM | 879 | CA | GLY | 1174 | 76.313 | 47.746 | 49.444 | 1.00 | 20.88 |
| ATOM | 880 | C | GLY | 1174 | 76.286 | 47.625 | 50.962 | 1.00 | 21.00 |
| ATOM | 881 | O | GLY | 1174 | 77.148 | 46.975 | 51.549 | 1.00 | 22.80 |
| ATOM | 882 | N | HIS | 1175 | 75.310 | 48.261 | 51.599 | 1.00 | 20.13 |
| ATOM | 883 | CA | HIS | 1175 | 75.170 | 48.218 | 53.052 | 1.00 | 19.74 |
| ATOM | 884 | CB | HIS | 1175 | 74.585 | 49.533 | 53.569 | 1.00 | 20.08 |
| ATOM | 885 | CG | HIS | 1175 | 75.465 | 50.726 | 53.336 | 1.00 | 21.55 |
| ATOM | 886 | CD2 | HIS | 1175 | 76.660 | 50.845 | 52.714 | 1.00 | 23.16 |
| ATOM | 887 | ND1 | HIS | 1175 | 75.134 | 51.990 | 53.775 | 1.00 | 22.98 |
| ATOM | 888 | CE1 | HIS | 1175 | 76.088 | 52.837 | 53.433 | 1.00 | 23.40 |
| ATOM | 889 | NE2 | HIS | 1175 | 77.026 | 52.168 | 52.787 | 1.00 | 22.42 |
| ATOM | 890 | C | HIS | 1175 | 74.277 | 47.049 | 53.481 | 1.00 | 20.52 |
| ATOM | 891 | O | HIS | 1175 | 73.344 | 46.679 | 52.770 | 1.00 | 21.87 |
| ATOM | 892 | N | ALA | 1176 | 74.553 | 46.492 | 54.653 | 1.00 | 19.06 |
| ATOM | 893 | CA | ALA | 1176 | 73.809 | 45.362 | 55.182 | 1.00 | 18.89 |
| ATOM | 894 | CB | ALA | 1176 | 74.470 | 44.863 | 56.442 | 1.00 | 18.59 |
| ATOM | 895 | C | ALA | 1176 | 72.353 | 45.643 | 55.475 | 1.00 | 21.37 |
| ATOM | 896 | O | ALA | 1176 | 72.031 | 46.496 | 56.304 | 1.00 | 21.49 |
| ATOM | 897 | N | VAL | 1177 | 71.473 | 44.897 | 54.817 | 1.00 | 22.39 |
| ATOM | 898 | CA | VAL | 1177 | 70.035 | 45.024 | 55.023 | 1.00 | 21.72 |
| ATOM | 899 | CB | VAL | 1177 | 69.246 | 44.821 | 53.703 | 1.00 | 22.74 |
| ATOM | 900 | CG1 | VAL | 1177 | 67.741 | 44.788 | 53.975 | 1.00 | 22.68 |
| ATOM | 901 | CG2 | VAL | 1177 | 69.582 | 45.930 | 52.720 | 1.00 | 20.67 |
| ATOM | 902 | C | VAL | 1177 | 69.634 | 43.949 | 56.027 | 1.00 | 21.01 |
| ATOM | 903 | O | VAL | 1177 | 68.814 | 44.182 | 56.915 | 1.00 | 22.35 |
| ATOM | 904 | N | GLY | 1178 | 70.245 | 42.777 | 55.891 | 1.00 | 20.58 |
| ATOM | 905 | CA | GLY | 1178 | 69.968 | 41.668 | 56.782 | 1.00 | 19.29 |
| ATOM | 906 | C | GLY | 1178 | 70.865 | 40.491 | 56.460 | 1.00 | 20.72 |
| ATOM | 907 | O | GLY | 1178 | 71.693 | 40.564 | 55.545 | 1.00 | 20.77 |
| ATOM | 908 | N | LEU | 1179 | 70.752 | 39.436 | 57.260 | 1.00 | 23.38 |
| ATOM | 909 | CA | LEU | 1179 | 71.521 | 38.208 | 57.066 | 1.00 | 24.90 |
| ATOM | 910 | CB | LEU | 1179 | 72.001 | 37.651 | 58.408 | 1.00 | 27.14 |
| ATOM | 911 | CG | LEU | 1179 | 73.435 | 37.842 | 58.896 | 1.00 | 27.77 |
| ATOM | 912 | CD1 | LEU | 1179 | 73.765 | 39.313 | 58.996 | 1.00 | 29.16 |

FIGURE 3 (CONT.)

| ATOM | 913 | CD2 | LEU | 1179 | 73.573 | 37.177 | 60.250 | 1.00 | 27.55 |
|------|-----|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 914 | C | LEU | 1179 | 70.578 | 37.189 | 56.461 | 1.00 | 25.10 |
| ATOM | 915 | O | LEU | 1179 | 69.475 | 37.000 | 56.964 | 1.00 | 26.82 |
| ATOM | 916 | N | PHE | 1180 | 70.987 | 36.552 | 55.375 | 1.00 | 25.52 |
| ATOM | 917 | CA | PHE | 1180 | 70.163 | 35.536 | 54.744 | 1.00 | 26.02 |
| ATOM | 918 | CB | PHE | 1180 | 70.861 | 35.030 | 53.485 | 1.00 | 26.33 |
| ATOM | 919 | CG | PHE | 1180 | 70.193 | 33.858 | 52.841 | 1.00 | 25.63 |
| ATOM | 920 | CD1 | PHE | 1180 | 68.809 | 33.754 | 52.804 | 1.00 | 24.18 |
| ATOM | 921 | CD2 | PHE | 1180 | 70.961 | 32.855 | 52.258 | 1.00 | 26.86 |
| ATOM | 922 | CE1 | PHE | 1180 | 68.203 | 32.669 | 52.196 | 1.00 | 26.34 |
| ATOM | 923 | CE2 | PHE | 1180 | 70.359 | 31.760 | 51.646 | 1.00 | 28.46 |
| ATOM | 924 | CZ | PHE | 1180 | 68.978 | 31.667 | 51.614 | 1.00 | 27.68 |
| ATOM | 925 | C | PHE | 1180 | 69.947 | 34.403 | 55.751 | 1.00 | 27.04 |
| ATOM | 926 | O | PHE | 1180 | 70.904 | 33.763 | 56.200 | 1.00 | 28.87 |
| ATOM | 927 | N | ARG | 1181 | 68.692 | 34.197 | 56.135 | 1.00 | 27.75 |
| ATOM | 928 | CA | ARG | 1181 | 68.335 | 33.168 | 57.105 | 1.00 | 28.04 |
| ATOM | 929 | CB | ARG | 1181 | 67.193 | 33.647 | 58.014 | 1.00 | 28.31 |
| ATOM | 930 | CG | ARG | 1181 | 66.773 | 32.609 | 59.047 | 1.00 | 30.17 |
| ATOM | 931 | CD | ARG | 1181 | 65.340 | 32.795 | 59.494 | 1.00 | 33.18 |
| ATOM | 932 | NE | ARG | 1181 | 65.225 | 33.558 | 60.730 | 1.00 | 37.63 |
| ATOM | 933 | CZ | ARG | 1181 | 64.538 | 34.694 | 60.858 | 1.00 | 40.99 |
| ATOM | 934 | NH1 | ARG | 1181 | 63.900 | 35.226 | 59.818 | 1.00 | 40.68 |
| ATOM | 935 | NH2 | ARG | 1181 | 64.455 | 35.281 | 62.048 | 1.00 | 42.67 |
| ATOM | 936 | C | ARG | 1181 | 67.962 | 31.827 | 56.477 | 1.00 | 28.46 |
| ATOM | 937 | O | ARG | 1181 | 68.499 | 30.784 | 56.872 | 1.00 | 30.26 |
| ATOM | 938 | N | ALA | 1182 | 67.046 | 31.838 | 55.514 | 1.00 | 27.65 |
| ATOM | 939 | CA | ALA | 1182 | 66.637 | 30.589 | 54.887 | 1.00 | 26.77 |
| ATOM | 940 | CB | ALA | 1182 | 65.686 | 29.841 | 55.794 | 1.00 | 28.57 |
| ATOM | 941 | C | ALA | 1182 | 66.002 | 30.777 | 53.529 | 1.00 | 26.90 |
| ATOM | 942 | O | ALA | 1182 | 65.457 | 31.842 | 53.223 | 1.00 | 24.79 |
| ATOM | 943 | N | ALA | 1183 | 66.085 | 29.727 | 52.720 | 1.00 | 27.64 |
| ATOM | 944 | CA | ALA | 1183 | 65.519 | 29.714 | 51.382 | 1.00 | 29.29 |
| ATOM | 945 | CB | ALA | 1183 | 66.356 | 28.821 | 50.469 | 1.00 | 28.99 |
| ATOM | 946 | C | ALA | 1183 | 64.080 | 29.207 | 51.433 | 1.00 | 31.69 |
| ATOM | 947 | O | ALA | 1183 | 63.803 | 28.136 | 51.992 | 1.00 | 31.90 |
| ATOM | 948 | N | VAL | 1184 | 63.170 | 30.012 | 50.893 | 1.00 | 32.81 |
| ATOM | 949 | CA | VAL | 1184 | 61.751 | 29.681 | 50.833 | 1.00 | 32.42 |
| ATOM | 950 | CB | VAL | 1184 | 60.893 | 30.928 | 51.005 | 1.00 | 30.12 |
| ATOM | 951 | CG1 | VAL | 1184 | 59.440 | 30.583 | 50.781 | 1.00 | 32.26 |
| ATOM | 952 | CG2 | VAL | 1184 | 61.106 | 31.522 | 52.380 | 1.00 | 30.64 |
| ATOM | 953 | C | VAL | 1184 | 61.498 | 29.131 | 49.441 | 1.00 | 33.36 |
| ATOM | 954 | O | VAL | 1184 | 61.370 | 29.894 | 48.478 | 1.00 | 32.09 |
| ATOM | 955 | N | CYS | 1185 | 61.403 | 27.816 | 49.326 | 1.00 | 35.08 |
| ATOM | 956 | CA | CYS | 1185 | 61.211 | 27.215 | 48.017 | 1.00 | 39.13 |
| ATOM | 957 | CB | CYS | 1185 | 62.486 | 26.482 | 47.601 | 1.00 | 41.48 |
| ATOM | 958 | SG | CYS | 1185 | 63.419 | 25.872 | 48.998 | 1.00 | 44.16 |
| ATOM | 959 | C | CYS | 1185 | 60.020 | 26.297 | 47.822 | 1.00 | 38.16 |
| ATOM | 960 | O | CYS | 1185 | 59.487 | 25.720 | 48.772 | 1.00 | 36.83 |
| ATOM | 961 | N | THR | 1186 | 59.574 | 26.236 | 46.571 | 1.00 | 38.73 |
| ATOM | 962 | CA | THR | 1186 | 58.469 | 25.385 | 46.185 | 1.00 | 37.64 |
| ATOM | 963 | CB | THR | 1186 | 57.582 | 26.052 | 45.133 | 1.00 | 33.24 |

FIGURE 3 (CONT.)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 964 | OG1 | THR | 1186 | 57.162 | 27.327 | 45.617 | 1.00 | 31.32 |
| ATOM | 965 | CG2 | THR | 1186 | 56.340 | 25.228 | 44.896 | 1.00 | 35.61 |
| ATOM | 966 | C | THR | 1186 | 59.040 | 24.049 | 45.703 | 1.00 | 40.01 |
| ATOM | 967 | O | THR | 1186 | 59.763 | 23.394 | 46.453 | 1.00 | 43.80 |
| ATOM | 968 | N | ARG | 1187 | 58.815 | 23.666 | 44.454 | 1.00 | 40.59 |
| ATOM | 969 | CA | ARG | 1187 | 59.313 | 22.371 | 44.016 | 1.00 | 42.08 |
| ATOM | 970 | CB | ARG | 1187 | 58.452 | 21.812 | 42.879 | 1.00 | 44.63 |
| ATOM | 971 | CG | ARG | 1187 | 56.993 | 21.591 | 43.280 | 1.00 | 45.00 |
| ATOM | 972 | CD | ARG | 1187 | 56.253 | 20.703 | 42.298 | 1.00 | 45.42 |
| ATOM | 973 | NE | ARG | 1187 | 56.736 | 19.327 | 42.361 | 1.00 | 47.14 |
| ATOM | 974 | CZ | ARG | 1187 | 57.309 | 18.683 | 41.348 | 1.00 | 48.66 |
| ATOM | 975 | NH1 | ARG | 1187 | 57.475 | 19.287 | 40.175 | 1.00 | 49.91 |
| ATOM | 976 | NH2 | ARG | 1187 | 57.731 | 17.433 | 41.511 | 1.00 | 49.91 |
| ATOM | 977 | C | ARG | 1187 | 60.788 | 22.349 | 43.668 | 1.00 | 42.04 |
| ATOM | 978 | O | ARG | 1187 | 61.165 | 22.021 | 42.545 | 1.00 | 44.12 |
| ATOM | 979 | N | GLY | 1188 | 61.623 | 22.687 | 44.647 | 1.00 | 41.58 |
| ATOM | 980 | CA | GLY | 1188 | 63.060 | 22.692 | 44.435 | 1.00 | 40.35 |
| ATOM | 981 | C | GLY | 1188 | 63.591 | 24.022 | 43.935 | 1.00 | 39.09 |
| ATOM | 982 | O | GLY | 1188 | 64.800 | 24.235 | 43.881 | 1.00 | 40.73 |
| ATOM | 983 | N | VAL | 1189 | 62.692 | 24.921 | 43.561 | 1.00 | 36.60 |
| ATOM | 984 | CA | VAL | 1189 | 63.097 | 26.220 | 43.069 | 1.00 | 35.55 |
| ATOM | 985 | CB | VAL | 1189 | 62.290 | 26.614 | 41.837 | 1.00 | 34.59 |
| ATOM | 986 | CG1 | VAL | 1189 | 62.634 | 28.026 | 41.401 | 1.00 | 36.44 |
| ATOM | 987 | CG2 | VAL | 1189 | 62.579 | 25.646 | 40.716 | 1.00 | 35.37 |
| ATOM | 988 | C | VAL | 1189 | 62.928 | 27.276 | 44.145 | 1.00 | 36.38 |
| ATOM | 989 | O | VAL | 1189 | 61.834 | 27.450 | 44.677 | 1.00 | 37.93 |
| ATOM | 990 | N | ALA | 1190 | 64.027 | 27.928 | 44.510 | 1.00 | 35.83 |
| ATOM | 991 | CA | ALA | 1190 | 64.002 | 28.983 | 45.513 | 1.00 | 34.95 |
| ATOM | 992 | CB | ALA | 1190 | 65.400 | 29.240 | 46.045 | 1.00 | 34.41 |
| ATOM | 993 | C | ALA | 1190 | 63.465 | 30.228 | 44.827 | 1.00 | 35.05 |
| ATOM | 994 | O | ALA | 1190 | 64.062 | 30.715 | 43.865 | 1.00 | 35.76 |
| ATOM | 995 | N | LYS | 1191 | 62.321 | 30.717 | 45.292 | 1.00 | 34.34 |
| ATOM | 996 | CA | LYS | 1191 | 61.710 | 31.907 | 44.709 | 1.00 | 33.55 |
| ATOM | 997 | CB | LYS | 1191 | 60.252 | 31.636 | 44.321 | 1.00 | 36.37 |
| ATOM | 998 | CG | LYS | 1191 | 60.037 | 30.443 | 43.404 | 1.00 | 38.02 |
| ATOM | 999 | CD | LYS | 1191 | 58.577 | 30.318 | 43.028 | 1.00 | 41.03 |
| ATOM | 1000 | CE | LYS | 1191 | 58.333 | 29.133 | 42.108 | 1.00 | 45.01 |
| ATOM | 1001 | NZ | LYS | 1191 | 56.902 | 29.078 | 41.674 | 1.00 | 45.80 |
| ATOM | 1002 | C | LYS | 1191 | 61.761 | 33.071 | 45.692 | 1.00 | 33.05 |
| ATOM | 1003 | O | LYS | 1191 | 61.652 | 34.231 | 45.298 | 1.00 | 36.29 |
| ATOM | 1004 | N | ALA | 1192 | 61.896 | 32.767 | 46.976 | 1.00 | 30.97 |
| ATOM | 1005 | CA | ALA | 1192 | 61.955 | 33.809 | 47.985 | 1.00 | 28.85 |
| ATOM | 1006 | CB | ALA | 1192 | 60.615 | 33.971 | 48.684 | 1.00 | 28.99 |
| ATOM | 1007 | C | ALA | 1192 | 63.051 | 33.494 | 48.984 | 1.00 | 28.42 |
| ATOM | 1008 | O | ALA | 1192 | 63.596 | 32.384 | 49.009 | 1.00 | 27.40 |
| ATOM | 1009 | N | VAL | 1193 | 63.299 | 34.452 | 49.863 | 1.00 | 27.93 |
| ATOM | 1010 | CA | VAL | 1193 | 64.355 | 34.356 | 50.847 | 1.00 | 27.23 |
| ATOM | 1011 | CB | VAL | 1193 | 65.569 | 35.180 | 50.329 | 1.00 | 27.43 |
| ATOM | 1012 | CG1 | VAL | 1193 | 66.002 | 36.251 | 51.317 | 1.00 | 26.78 |
| ATOM | 1013 | CG2 | VAL | 1193 | 66.696 | 34.258 | 49.948 | 1.00 | 26.32 |
| ATOM | 1014 | C | VAL | 1193 | 63.858 | 34.863 | 52.204 | 1.00 | 28.65 |

23/60

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1015 | O | VAL | 1193 | 63.059 | 35.803 | 52.281 | 1.00 | 29.70 |
| ATOM | 1016 | N | ASP | 1194 | 64.336 | 34.233 | 53.268 | 1.00 | 29.83 |
| ATOM | 1017 | CA | ASP | 1194 | 63.961 | 34.593 | 54.634 | 1.00 | 31.77 |
| ATOM | 1018 | CB | ASP | 1194 | 63.611 | 33.308 | 55.403 | 1.00 | 35.32 |
| ATOM | 1019 | CG | ASP | 1194 | 62.533 | 33.513 | 56.461 | 1.00 | 39.12 |
| ATOM | 1020 | OD1 | ASP | 1194 | 62.701 | 32.961 | 57.574 | 1.00 | 40.47 |
| ATOM | 1021 | OD2 | ASP | 1194 | 61.508 | 34.176 | 56.169 | 1.00 | 39.60 |
| ATOM | 1022 | C | ASP | 1194 | 65.218 | 35.227 | 55.226 | 1.00 | 29.50 |
| ATOM | 1023 | O | ASP | 1194 | 66.317 | 34.724 | 54.995 | 1.00 | 30.45 |
| ATOM | 1024 | N | PHE | 1195 | 65.092 | 36.322 | 55.966 | 1.00 | 27.58 |
| ATOM | 1025 | CA | PHE | 1195 | 66.292 | 36.927 | 56.537 | 1.00 | 25.93 |
| ATOM | 1026 | CB | PHE | 1195 | 66.981 | 37.869 | 55.532 | 1.00 | 21.65 |
| ATOM | 1027 | CG | PHE | 1195 | 66.204 | 39.118 | 55.204 | 1.00 | 17.29 |
| ATOM | 1028 | CD1 | PHE | 1195 | 66.358 | 40.267 | 55.969 | 1.00 | 17.07 |
| ATOM | 1029 | CD2 | PHE | 1195 | 65.363 | 39.162 | 54.100 | 1.00 | 17.69 |
| ATOM | 1030 | CE1 | PHE | 1195 | 65.689 | 41.447 | 55.644 | 1.00 | 17.82 |
| ATOM | 1031 | CE2 | PHE | 1195 | 64.685 | 40.343 | 53.761 | 1.00 | 19.76 |
| ATOM | 1032 | CZ | PHE | 1195 | 64.849 | 41.491 | 54.538 | 1.00 | 18.59 |
| ATOM | 1033 | C | PHE | 1195 | 66.140 | 37.590 | 57.897 | 1.00 | 25.99 |
| ATOM | 1034 | O | PHE | 1195 | 65.034 | 37.746 | 58.404 | 1.00 | 27.20 |
| ATOM | 1035 | N | ILE | 1196 | 67.283 | 37.916 | 58.496 | 1.00 | 26.69 |
| ATOM | 1036 | CA | ILE | 1196 | 67.389 | 38.562 | 59.804 | 1.00 | 25.40 |
| ATOM | 1037 | CB | ILE | 1196 | 68.535 | 37.900 | 60.617 | 1.00 | 23.91 |
| ATOM | 1038 | CG2 | ILE | 1196 | 68.599 | 38.457 | 62.027 | 1.00 | 22.64 |
| ATOM | 1039 | CG1 | ILE | 1196 | 68.357 | 36.381 | 60.645 | 1.00 | 20.68 |
| ATOM | 1040 | CD1 | ILE | 1196 | 69.570 | 35.656 | 61.152 | 1.00 | 20.36 |
| ATOM | 1041 | C | ILE | 1196 | 67.777 | 40.026 | 59.548 | 1.00 | 28.07 |
| ATOM | 1042 | O | ILE | 1196 | 68.907 | 40.309 | 59.147 | 1.00 | 31.19 |
| ATOM | 1043 | N | PRO | 1197 | 66.853 | 40.972 | 59.757 | 1.00 | 28.04 |
| ATOM | 1044 | CD | PRO | 1197 | 65.466 | 40.830 | 60.225 | 1.00 | 27.62 |
| ATOM | 1045 | CA | PRO | 1197 | 67.187 | 42.382 | 59.521 | 1.00 | 29.04 |
| ATOM | 1046 | CB | PRO | 1197 | 65.851 | 43.087 | 59.764 | 1.00 | 27.29 |
| ATOM | 1047 | CG | PRO | 1197 | 65.177 | 42.204 | 60.758 | 1.00 | 27.91 |
| ATOM | 1048 | C | PRO | 1197 | 68.296 | 42.924 | 60.437 | 1.00 | 30.39 |
| ATOM | 1049 | O | PRO | 1197 | 68.445 | 42.469 | 61.571 | 1.00 | 30.42 |
| ATOM | 1050 | N | VAL | 1198 | 69.060 | 43.904 | 59.950 | 1.00 | 32.28 |
| ATOM | 1051 | CA | VAL | 1198 | 70.149 | 44.497 | 60.738 | 1.00 | 32.71 |
| ATOM | 1052 | CB | VAL | 1198 | 70.968 | 45.569 | 59.977 | 1.00 | 31.13 |
| ATOM | 1053 | CG1 | VAL | 1198 | 71.893 | 44.906 | 58.992 | 1.00 | 32.44 |
| ATOM | 1054 | CG2 | VAL | 1198 | 70.060 | 46.576 | 59.294 | 1.00 | 30.27 |
| ATOM | 1055 | C | VAL | 1198 | 69.706 | 45.106 | 62.046 | 1.00 | 33.07 |
| ATOM | 1056 | O | VAL | 1198 | 70.494 | 45.192 | 62.982 | 1.00 | 34.24 |
| ATOM | 1057 | N | GLU | 1199 | 68.459 | 45.557 | 62.112 | 1.00 | 34.76 |
| ATOM | 1058 | CA | GLU | 1199 | 67.942 | 46.133 | 63.348 | 1.00 | 35.58 |
| ATOM | 1059 | CB | GLU | 1199 | 66.502 | 46.601 | 63.167 | 1.00 | 38.30 |
| ATOM | 1060 | CG | GLU | 1199 | 66.347 | 47.817 | 62.251 | 1.00 | 43.36 |
| ATOM | 1061 | CD | GLU | 1199 | 66.682 | 47.546 | 60.781 | 1.00 | 44.71 |
| ATOM | 1062 | OE1 | GLU | 1199 | 67.295 | 48.437 | 60.157 | 1.00 | 46.89 |
| ATOM | 1063 | OE2 | GLU | 1199 | 66.319 | 46.470 | 60.248 | 1.00 | 43.96 |
| ATOM | 1064 | C | GLU | 1199 | 68.035 | 45.092 | 64.465 | 1.00 | 35.11 |
| ATOM | 1065 | O | GLU | 1199 | 68.357 | 45.424 | 65.599 | 1.00 | 35.89 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1066 | N | ASN | 1200 | 67.827 | 43.823 | 64.126 | 1.00 | 34.53 |
| ATOM | 1067 | CA | ASN | 1200 | 67.918 | 42.750 | 65.108 | 1.00 | 34.98 |
| ATOM | 1068 | CB | ASN | 1200 | 67.515 | 41.414 | 64.486 | 1.00 | 36.70 |
| ATOM | 1069 | CG | ASN | 1200 | 66.017 | 41.289 | 64.286 | 1.00 | 40.49 |
| ATOM | 1070 | OD1 | ASN | 1200 | 65.442 | 40.231 | 64.528 | 1.00 | 43.89 |
| ATOM | 1071 | ND2 | ASN | 1200 | 65.377 | 42.358 | 63.827 | 1.00 | 40.79 |
| ATOM | 1072 | C | ASN | 1200 | 69.345 | 42.663 | 65.640 | 1.00 | 35.32 |
| ATOM | 1073 | O | ASN | 1200 | 69.561 | 42.654 | 66.852 | 1.00 | 35.57 |
| ATOM | 1074 | N | LEU | 1201 | 70.319 | 42.635 | 64.733 | 1.00 | 34.45 |
| ATOM | 1075 | CA | LEU | 1201 | 71.727 | 42.568 | 65.124 | 1.00 | 32.80 |
| ATOM | 1076 | CB | LEU | 1201 | 72.643 | 42.631 | 63.900 | 1.00 | 31.13 |
| ATOM | 1077 | CG | LEU | 1201 | 72.856 | 41.383 | 63.053 | 1.00 | 30.40 |
| ATOM | 1078 | CD1 | LEU | 1201 | 71.547 | 40.751 | 62.648 | 1.00 | 31.05 |
| ATOM | 1079 | CD2 | LEU | 1201 | 73.654 | 41.764 | 61.833 | 1.00 | 30.17 |
| ATOM | 1080 | C | LEU | 1201 | 72.026 | 43.749 | 66.028 | 1.00 | 33.31 |
| ATOM | 1081 | O | LEU | 1201 | 72.535 | 43.585 | 67.135 | 1.00 | 33.72 |
| ATOM | 1082 | N | GLU | 1202 | 71.653 | 44.933 | 65.558 | 1.00 | 33.90 |
| ATOM | 1083 | CA | GLU | 1202 | 71.861 | 46.171 | 66.294 | 1.00 | 35.75 |
| ATOM | 1084 | CB | GLU | 1202 | 71.292 | 47.351 | 65.500 | 1.00 | 34.70 |
| ATOM | 1085 | CG | GLU | 1202 | 72.029 | 47.574 | 64.190 | 1.00 | 37.02 |
| ATOM | 1086 | CD | GLU | 1202 | 71.347 | 48.547 | 63.247 | 1.00 | 40.33 |
| ATOM | 1087 | OE1 | GLU | 1202 | 71.990 | 48.934 | 62.256 | 1.00 | 43.28 |
| ATOM | 1088 | OE2 | GLU | 1202 | 70.175 | 48.924 | 63.462 | 1.00 | 44.53 |
| ATOM | 1089 | C | GLU | 1202 | 71.285 | 46.122 | 67.713 | 1.00 | 37.01 |
| ATOM | 1090 | O | GLU | 1202 | 71.977 | 46.459 | 68.673 | 1.00 | 38.58 |
| ATOM | 1091 | N | THR | 1203 | 70.043 | 45.672 | 67.855 | 1.00 | 36.83 |
| ATOM | 1092 | CA | THR | 1203 | 69.435 | 45.592 | 69.174 | 1.00 | 38.22 |
| ATOM | 1093 | CB | THR | 1203 | 67.956 | 45.209 | 69.099 | 1.00 | 38.67 |
| ATOM | 1094 | OG1 | THR | 1203 | 67.828 | 43.951 | 68.434 | 1.00 | 42.02 |
| ATOM | 1095 | CG2 | THR | 1203 | 67.168 | 46.264 | 68.352 | 1.00 | 38.87 |
| ATOM | 1096 | C | THR | 1203 | 70.156 | 44.548 | 70.001 | 1.00 | 39.56 |
| ATOM | 1097 | O | THR | 1203 | 70.425 | 44.764 | 71.180 | 1.00 | 40.65 |
| ATOM | 1098 | N | THR | 1204 | 70.479 | 43.421 | 69.370 | 1.00 | 40.29 |
| ATOM | 1099 | CA | THR | 1204 | 71.180 | 42.328 | 70.040 | 1.00 | 40.51 |
| ATOM | 1100 | CB | THR | 1204 | 71.409 | 41.146 | 69.075 | 1.00 | 39.96 |
| ATOM | 1101 | OG1 | THR | 1204 | 70.150 | 40.520 | 68.785 | 1.00 | 37.72 |
| ATOM | 1102 | CG2 | THR | 1204 | 72.353 | 40.120 | 69.677 | 1.00 | 41.21 |
| ATOM | 1103 | C | THR | 1204 | 72.492 | 42.818 | 70.648 | 1.00 | 41.33 |
| ATOM | 1104 | O | THR | 1204 | 72.932 | 42.322 | 71.684 | 1.00 | 42.16 |
| ATOM | 1105 | N | MET | 1205 | 73.101 | 43.810 | 70.012 | 1.00 | 42.92 |
| ATOM | 1106 | CA | MET | 1205 | 74.338 | 44.395 | 70.510 | 1.00 | 44.88 |
| ATOM | 1107 | CB | MET | 1205 | 75.064 | 45.136 | 69.388 | 1.00 | 43.43 |
| ATOM | 1108 | CG | MET | 1205 | 75.778 | 44.265 | 68.388 | 1.00 | 41.30 |
| ATOM | 1109 | SD | MET | 1205 | 76.649 | 45.304 | 67.195 | 1.00 | 38.98 |
| ATOM | 1110 | CE | MET | 1205 | 75.690 | 45.025 | 65.732 | 1.00 | 39.73 |
| ATOM | 1111 | C | MET | 1205 | 74.008 | 45.401 | 71.612 | 1.00 | 48.30 |
| ATOM | 1112 | O | MET | 1205 | 74.680 | 46.434 | 71.732 | 1.00 | 50.45 |
| ATOM | 1113 | N | ALA | 1206 | 72.985 | 45.106 | 72.415 | 1.00 | 51.29 |
| ATOM | 1114 | CA | ALA | 1206 | 72.560 | 46.001 | 73.494 | 1.00 | 52.72 |
| ATOM | 1115 | CB | ALA | 1206 | 71.741 | 47.167 | 72.919 | 1.00 | 51.79 |
| ATOM | 1116 | C | ALA | 1206 | 71.746 | 45.253 | 74.550 | 1.00 | 52.50 |

| ATOM 1117 | O | ALA | 1206 | 70.842 | 44.487 | 74.147 | 1.00 | 52.28 |
|---|---|---|---|---|---|---|---|---|

### sNS4ACOORDINATES   (Complex A)

| Atom Type | Resid | # | X | Y | Z | OCC | B |
|---|---|---|---|---|---|---|---|
| ATOM 2427 | N | GLY | 1678 | 82.660 | 20.678 | 69.142 | 1.00 | 47.82 |
| ATOM 2428 | CA | GLY | 1678 | 83.325 | 21.195 | 67.901 | 1.00 | 47.45 |
| ATOM 2429 | C | GLY | 1678 | 83.444 | 22.729 | 67.863 | 1.00 | 42.58 |
| ATOM 2430 | O | GLY | 1678 | 83.086 | 23.435 | 68.815 | 1.00 | 46.32 |
| ATOM 2431 | N | SER | 1679 | 83.951 | 23.237 | 66.745 | 1.00 | 39.26 |
| ATOM 2432 | CA | SER | 1679 | 84.188 | 24.669 | 66.594 | 1.00 | 35.38 |
| ATOM 2433 | CB | SER | 1679 | 85.628 | 24.981 | 67.011 | 1.00 | 34.24 |
| ATOM 2434 | OG | SER | 1679 | 85.746 | 26.265 | 67.587 | 1.00 | 33.09 |
| ATOM 2435 | C | SER | 1679 | 83.965 | 25.057 | 65.134 | 1.00 | 32.76 |
| ATOM 2436 | O | SER | 1679 | 84.084 | 24.218 | 64.240 | 1.00 | 34.29 |
| ATOM 2437 | N | VAL | 1680 | 83.594 | 26.307 | 64.894 | 1.00 | 29.61 |
| ATOM 2438 | CA | VAL | 1680 | 83.365 | 26.784 | 63.533 | 1.00 | 27.92 |
| ATOM 2439 | CB | VAL | 1680 | 82.341 | 27.936 | 63.495 | 1.00 | 27.03 |
| ATOM 2440 | CG1 | VAL | 1680 | 81.995 | 28.277 | 62.069 | 1.00 | 26.39 |
| ATOM 2441 | CG2 | VAL | 1680 | 81.099 | 27.569 | 64.277 | 1.00 | 27.69 |
| ATOM 2442 | C | VAL | 1680 | 84.692 | 27.311 | 63.007 | 1.00 | 26.65 |
| ATOM 2443 | O | VAL | 1680 | 85.349 | 28.115 | 63.666 | 1.00 | 28.02 |
| ATOM 2444 | N | VAL | 1681 | 85.108 | 26.844 | 61.842 | 1.00 | 24.80 |
| ATOM 2445 | CA | VAL | 1681 | 86.364 | 27.300 | 61.278 | 1.00 | 23.49 |
| ATOM 2446 | CB | VAL | 1681 | 87.331 | 26.117 | 61.027 | 1.00 | 23.05 |
| ATOM 2447 | CG1 | VAL | 1681 | 87.591 | 25.384 | 62.314 | 1.00 | 21.97 |
| ATOM 2448 | CG2 | VAL | 1681 | 86.751 | 25.153 | 60.018 | 1.00 | 24.91 |
| ATOM 2449 | C | VAL | 1681 | 86.106 | 28.061 | 59.985 | 1.00 | 22.71 |
| ATOM 2450 | O | VAL | 1681 | 85.156 | 27.762 | 59.261 | 1.00 | 22.32 |
| ATOM 2451 | N | ILE | 1682 | 86.923 | 29.077 | 59.729 | 1.00 | 22.79 |
| ATOM 2452 | CA | ILE | 1682 | 86.809 | 29.899 | 58.528 | 1.00 | 19.66 |
| ATOM 2453 | CB | ILE | 1682 | 87.309 | 31.332 | 58.811 | 1.00 | 16.80 |
| ATOM 2454 | CG2 | ILE | 1682 | 87.324 | 32.164 | 57.540 | 1.00 | 16.76 |
| ATOM 2455 | CG1 | ILE | 1682 | 86.417 | 31.981 | 59.875 | 1.00 | 13.77 |
| ATOM 2456 | CD1 | ILE | 1682 | 86.965 | 33.244 | 60.432 | 1.00 | 9.56 |
| ATOM 2457 | C | ILE | 1682 | 87.627 | 29.247 | 57.418 | 1.00 | 19.97 |
| ATOM 2458 | O | ILE | 1682 | 88.844 | 29.115 | 57.522 | 1.00 | 20.81 |
| ATOM 2459 | N | VAL | 1683 | 86.946 | 28.826 | 56.361 | 1.00 | 20.17 |
| ATOM 2460 | CA | VAL | 1683 | 87.599 | 28.157 | 55.253 | 1.00 | 18.67 |
| ATOM 2461 | CB | VAL | 1683 | 86.827 | 26.867 | 54.857 | 1.00 | 20.13 |
| ATOM 2462 | CG1 | VAL | 1683 | 86.595 | 25.992 | 56.091 | 1.00 | 19.43 |
| ATOM 2463 | CG2 | VAL | 1683 | 85.511 | 27.205 | 54.188 | 1.00 | 21.44 |
| ATOM 2464 | C | VAL | 1683 | 87.785 | 29.039 | 54.027 | 1.00 | 17.87 |
| ATOM 2465 | O | VAL | 1683 | 88.279 | 28.592 | 52.993 | 1.00 | 19.88 |
| ATOM 2466 | N | GLY | 1684 | 87.400 | 30.297 | 54.135 | 1.00 | 16.04 |
| ATOM 2467 | CA | GLY | 1684 | 87.547 | 31.186 | 53.005 | 1.00 | 13.85 |
| ATOM 2468 | C | GLY | 1684 | 87.006 | 32.540 | 53.374 | 1.00 | 14.18 |
| ATOM 2469 | O | GLY | 1684 | 86.476 | 32.709 | 54.473 | 1.00 | 11.33 |
| ATOM 2470 | N | ARG | 1685 | 87.119 | 33.492 | 52.452 | 1.00 | 16.02 |

FIGURE 3 (CONT.)

| ATOM | 2471 | CA | ARG | 1685 | 86.660 | 34.861 | 52.660 | 1.00 | 16.38 |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 2472 | CB | ARG | 1685 | 87.800 | 35.715 | 53.219 | 1.00 | 17.53 |
| ATOM | 2473 | CG | ARG | 1685 | 88.339 | 35.249 | 54.559 | 1.00 | 18.90 |
| ATOM | 2474 | CD | ARG | 1685 | 89.566 | 36.039 | 54.945 | 1.00 | 20.79 |
| ATOM | 2475 | NE | ARG | 1685 | 90.609 | 35.890 | 53.940 | 1.00 | 21.09 |
| ATOM | 2476 | CZ | ARG | 1685 | 91.532 | 36.808 | 53.676 | 1.00 | 22.64 |
| ATOM | 2477 | NH1 | ARG | 1685 | 91.552 | 37.957 | 54.348 | 1.00 | 21.65 |
| ATOM | 2478 | NH2 | ARG | 1685 | 92.426 | 36.581 | 52.722 | 1.00 | 21.05 |
| ATOM | 2479 | C | ARG | 1685 | 86.180 | 35.460 | 51.343 | 1.00 | 15.81 |
| ATOM | 2480 | O | ARG | 1685 | 86.606 | 35.034 | 50.273 | 1.00 | 17.35 |
| ATOM | 2481 | N | ILE | 1686 | 85.313 | 36.464 | 51.432 | 1.00 | 14.82 |
| ATOM | 2482 | CA | ILE | 1686 | 84.761 | 37.142 | 50.267 | 1.00 | 13.14 |
| ATOM | 2483 | CB | ILE | 1686 | 83.249 | 36.799 | 50.100 | 1.00 | 14.91 |
| ATOM | 2484 | CG2 | ILE | 1686 | 82.530 | 37.816 | 49.216 | 1.00 | 9.50 |
| ATOM | 2485 | CG1 | ILE | 1686 | 83.098 | 35.380 | 49.543 | 1.00 | 16.63 |
| ATOM | 2486 | CD1 | ILE | 1686 | 81.686 | 34.958 | 49.338 | 1.00 | 16.16 |
| ATOM | 2487 | C | ILE | 1686 | 84.909 | 38.637 | 50.472 | 1.00 | 13.59 |
| ATOM | 2488 | O | ILE | 1686 | 84.614 | 39.142 | 51.549 | 1.00 | 14.05 |
| ATOM | 2489 | N | VAL | 1687 | 85.412 | 39.333 | 49.458 | 1.00 | 15.01 |
| ATOM | 2490 | CA | VAL | 1687 | 85.575 | 40.786 | 49.508 | 1.00 | 15.16 |
| ATOM | 2491 | CB | VAL | 1687 | 86.997 | 41.223 | 49.052 | 1.00 | 15.36 |
| ATOM | 2492 | CG1 | VAL | 1687 | 87.290 | 40.797 | 47.611 | 1.00 | 12.78 |
| ATOM | 2493 | CG2 | VAL | 1687 | 87.155 | 42.702 | 49.214 | 1.00 | 15.07 |
| ATOM | 2494 | C | VAL | 1687 | 84.500 | 41.372 | 48.588 | 1.00 | 16.77 |
| ATOM | 2495 | O | VAL | 1687 | 84.556 | 41.212 | 47.372 | 1.00 | 18.75 |
| ATOM | 2496 | N | LEU | 1688 | 83.500 | 42.017 | 49.174 | 1.00 | 16.57 |
| ATOM | 2497 | CA | LEU | 1688 | 82.394 | 42.576 | 48.411 | 1.00 | 16.18 |
| ATOM | 2498 | CB | LEU | 1688 | 81.400 | 43.254 | 49.344 | 1.00 | 15.30 |
| ATOM | 2499 | CG | LEU | 1688 | 80.742 | 42.326 | 50.369 | 1.00 | 14.41 |
| ATOM | 2500 | CD1 | LEU | 1688 | 79.737 | 43.122 | 51.173 | 1.00 | 12.70 |
| ATOM | 2501 | CD2 | LEU | 1688 | 80.083 | 41.142 | 49.672 | 1.00 | 10.09 |
| ATOM | 2502 | C | LEU | 1688 | 82.737 | 43.502 | 47.260 | 1.00 | 19.55 |
| ATOM | 2503 | O | LEU | 1688 | 82.047 | 43.504 | 46.243 | 1.00 | 23.25 |
| ATOM | 2504 | N | SER | 1689 | 83.803 | 44.277 | 47.401 | 1.00 | 23.03 |
| ATOM | 2505 | CA | SER | 1689 | 84.209 | 45.213 | 46.353 | 1.00 | 21.96 |
| ATOM | 2506 | CB | SER | 1689 | 84.999 | 46.366 | 46.968 | 1.00 | 21.45 |
| ATOM | 2507 | OG | SER | 1689 | 86.151 | 45.888 | 47.643 | 1.00 | 24.53 |
| ATOM | 2508 | C | SER | 1689 | 85.031 | 44.593 | 45.238 | 1.00 | 22.42 |
| ATOM | 2509 | O | SER | 1689 | 85.306 | 45.252 | 44.239 | 1.00 | 25.52 |
| ATOM | 2510 | N | GLY | 1690 | 85.430 | 43.337 | 45.409 | 1.00 | 21.46 |
| ATOM | 2511 | CA | GLY | 1690 | 86.242 | 42.676 | 44.406 | 1.00 | 21.23 |
| ATOM | 2512 | C | GLY | 1690 | 87.690 | 43.130 | 44.463 | 1.00 | 23.65 |
| ATOM | 2513 | O | GLY | 1690 | 88.451 | 42.922 | 43.521 | 1.00 | 25.98 |
| ATOM | 2514 | N | LYS | 1691 | 88.082 | 43.738 | 45.577 | 1.00 | 23.43 |
| ATOM | 2515 | CA | LYS | 1691 | 89.445 | 44.224 | 45.746 | 1.00 | 23.50 |
| ATOM | 2516 | CB | LYS | 1691 | 89.561 | 44.980 | 47.067 | 1.00 | 21.39 |
| ATOM | 2517 | CG | LYS | 1691 | 90.907 | 45.621 | 47.286 | 1.00 | 21.65 |
| ATOM | 2518 | CD | LYS | 1691 | 90.888 | 46.513 | 48.507 | 1.00 | 22.73 |
| ATOM | 2519 | CE | LYS | 1691 | 92.193 | 47.269 | 48.654 | 1.00 | 23.13 |
| ATOM | 2520 | NZ | LYS | 1691 | 92.079 | 48.318 | 49.700 | 1.00 | 27.11 |
| ATOM | 2521 | C | LYS | 1691 | 90.503 | 43.116 | 45.680 | 1.00 | 24.67 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM 2522 | O | LYS | 1691 | 90.440 | 42.133 | 46.424 | 1.00 | 26.46 |
| ATOM 2523 | N | PRO | 1692 | 91.475 | 43.249 | 44.765 | 1.00 | 25.07 |
| ATOM 2524 | CD | PRO | 1692 | 91.517 | 44.246 | 43.682 | 1.00 | 24.13 |
| ATOM 2525 | CA | PRO | 1692 | 92.549 | 42.270 | 44.598 | 1.00 | 25.54 |
| ATOM 2526 | CB | PRO | 1692 | 92.933 | 42.456 | 43.143 | 1.00 | 22.92 |
| ATOM 2527 | CG | PRO | 1692 | 92.815 | 43.920 | 42.986 | 1.00 | 23.88 |
| ATOM 2528 | C | PRO | 1692 | 93.716 | 42.601 | 45.516 | 1.00 | 27.60 |
| ATOM 2529 | O | PRO | 1692 | 93.810 | 43.716 | 46.029 | 1.00 | 29.48 |
| ATOM 2530 | N | ALA | 1693 | 94.570 | 41.620 | 45.770 | 1.00 | 31.04 |
| ATOM 2531 | CA | ALA | 1693 | 95.736 | 41.833 | 46.621 | 1.00 | 34.86 |
| ATOM 2532 | CB | ALA | 1693 | 96.112 | 40.543 | 47.326 | 1.00 | 35.21 |
| ATOM 2533 | C | ALA | 1693 | 96.915 | 42.354 | 45.798 | 1.00 | 35.37 |
| ATOM 2534 | O | ALA | 1693 | 96.891 | 42.145 | 44.559 | 1.00 | 35.58 |

## tNS3COORDINATES (ComplexB)

| | Atom Type | Resid | # | X | Y | Z | OCC | B |
|---|---|---|---|---|---|---|---|---|
| ATOM 1118 | N | PRO | 1028 | 74.820 | 45.651 | 43.675 | 1.00 | 28.69 |
| ATOM 1119 | CD | PRO | 1028 | 75.076 | 44.493 | 44.550 | 1.00 | 28.33 |
| ATOM 1120 | CA | PRO | 1028 | 74.869 | 46.897 | 44.441 | 1.00 | 28.80 |
| ATOM 1121 | CB | PRO | 1028 | 74.807 | 46.400 | 45.883 | 1.00 | 28.68 |
| ATOM 1122 | CG | PRO | 1028 | 75.597 | 45.138 | 45.819 | 1.00 | 27.37 |
| ATOM 1123 | C | PRO | 1028 | 76.163 | 47.662 | 44.173 | 1.00 | 28.69 |
| ATOM 1124 | O | PRO | 1028 | 77.141 | 47.094 | 43.666 | 1.00 | 30.88 |
| ATOM 1125 | N | ILE | 1029 | 76.172 | 48.950 | 44.500 | 1.00 | 25.65 |
| ATOM 1126 | CA | ILE | 1029 | 77.359 | 49.763 | 44.288 | 1.00 | 22.21 |
| ATOM 1127 | CB | ILE | 1029 | 77.029 | 51.251 | 44.319 | 1.00 | 19.66 |
| ATOM 1128 | CG2 | ILE | 1029 | 78.254 | 52.059 | 43.933 | 1.00 | 21.71 |
| ATOM 1129 | CG1 | ILE | 1029 | 75.883 | 51.554 | 43.355 | 1.00 | 19.62 |
| ATOM 1130 | CD1 | ILE | 1029 | 75.398 | 52.960 | 43.428 | 1.00 | 14.82 |
| ATOM 1131 | C | ILE | 1029 | 78.383 | 49.463 | 45.371 | 1.00 | 23.25 |
| ATOM 1132 | O | ILE | 1029 | 78.094 | 49.586 | 46.559 | 1.00 | 25.52 |
| ATOM 1133 | N | THR | 1030 | 79.561 | 49.023 | 44.951 | 1.00 | 23.20 |
| ATOM 1134 | CA | THR | 1030 | 80.651 | 48.725 | 45.860 | 1.00 | 23.22 |
| ATOM 1135 | CB | THR | 1030 | 80.916 | 47.207 | 45.958 | 1.00 | 23.28 |
| ATOM 1136 | OG1 | THR | 1030 | 81.077 | 46.659 | 44.641 | 1.00 | 27.79 |
| ATOM 1137 | CG2 | THR | 1030 | 79.764 | 46.508 | 46.652 | 1.00 | 24.32 |
| ATOM 1138 | C | THR | 1030 | 81.879 | 49.406 | 45.277 | 1.00 | 23.10 |
| ATOM 1139 | O | THR | 1030 | 81.982 | 49.562 | 44.059 | 1.00 | 24.23 |
| ATOM 1140 | N | ALA | 1031 | 82.821 | 49.779 | 46.134 | 1.00 | 20.99 |
| ATOM 1141 | CA | ALA | 1031 | 84.024 | 50.456 | 45.675 | 1.00 | 18.06 |
| ATOM 1142 | CB | ALA | 1031 | 83.776 | 51.946 | 45.635 | 1.00 | 19.68 |
| ATOM 1143 | C | ALA | 1031 | 85.205 | 50.172 | 46.579 | 1.00 | 17.02 |
| ATOM 1144 | O | ALA | 1031 | 85.036 | 49.858 | 47.751 | 1.00 | 17.50 |
| ATOM 1145 | N | TYR | 1032 | 86.404 | 50.250 | 46.028 | 1.00 | 16.80 |
| ATOM 1146 | CA | TYR | 1032 | 87.597 | 50.064 | 46.837 | 1.00 | 18.55 |
| ATOM 1147 | CB | TYR | 1032 | 88.127 | 48.633 | 46.786 | 1.00 | 18.83 |
| ATOM 1148 | CG | TYR | 1032 | 88.710 | 48.185 | 45.466 | 1.00 | 15.88 |
| ATOM 1149 | CD1 | TYR | 1032 | 89.997 | 48.545 | 45.088 | 1.00 | 13.44 |

FIGURE 3 (CONT.)

| ATOM | 1150 | CE1 | TYR | 1032 | 90.540 | 48.083 | 43.899 | 1.00 | 15.11 |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 1151 | CD2 | TYR | 1032 | 87.982 | 47.360 | 44.619 | 1.00 | 15.92 |
| ATOM | 1152 | CE2 | TYR | 1032 | 88.514 | 46.893 | 43.436 | 1.00 | 15.01 |
| ATOM | 1153 | CZ | TYR | 1032 | 89.788 | 47.255 | 43.075 | 1.00 | 15.25 |
| ATOM | 1154 | OH | TYR | 1032 | 90.298 | 46.766 | 41.894 | 1.00 | 16.61 |
| ATOM | 1155 | C | TYR | 1032 | 88.645 | 51.045 | 46.368 | 1.00 | 18.69 |
| ATOM | 1156 | O | TYR | 1032 | 88.632 | 51.462 | 45.211 | 1.00 | 19.25 |
| ATOM | 1157 | N | ALA | 1033 | 89.525 | 51.443 | 47.274 | 1.00 | 19.62 |
| ATOM | 1158 | CA | ALA | 1033 | 90.567 | 52.394 | 46.944 | 1.00 | 20.61 |
| ATOM | 1159 | CB | ALA | 1033 | 90.539 | 53.545 | 47.922 | 1.00 | 18.51 |
| ATOM | 1160 | C | ALA | 1033 | 91.941 | 51.738 | 46.933 | 1.00 | 22.70 |
| ATOM | 1161 | O | ALA | 1033 | 92.142 | 50.670 | 47.525 | 1.00 | 24.65 |
| ATOM | 1162 | N | GLN | 1034 | 92.869 | 52.361 | 46.215 | 1.00 | 23.10 |
| ATOM | 1163 | CA | GLN | 1034 | 94.236 | 51.880 | 46.120 | 1.00 | 21.69 |
| ATOM | 1164 | CB | GLN | 1034 | 94.432 | 50.971 | 44.899 | 1.00 | 22.35 |
| ATOM | 1165 | CG | GLN | 1034 | 93.643 | 49.679 | 44.895 | 1.00 | 23.27 |
| ATOM | 1166 | CD | GLN | 1034 | 93.927 | 48.834 | 43.666 | 1.00 | 26.53 |
| ATOM | 1167 | OE1 | GLN | 1034 | 93.982 | 49.341 | 42.544 | 1.00 | 27.77 |
| ATOM | 1168 | NE2 | GLN | 1034 | 94.119 | 47.537 | 43.872 | 1.00 | 27.16 |
| ATOM | 1169 | C | GLN | 1034 | 95.111 | 53.103 | 45.955 | 1.00 | 22.49 |
| ATOM | 1170 | O | GLN | 1034 | 94.780 | 54.005 | 45.186 | 1.00 | 21.85 |
| ATOM | 1171 | N | GLN | 1035 | 96.194 | 53.156 | 46.722 | 1.00 | 25.39 |
| ATOM | 1172 | CA | GLN | 1035 | 97.151 | 54.253 | 46.648 | 1.00 | 26.92 |
| ATOM | 1173 | CB | GLN | 1035 | 97.779 | 54.498 | 48.013 | 1.00 | 29.66 |
| ATOM | 1174 | CG | GLN | 1035 | 98.985 | 55.414 | 47.971 | 1.00 | 37.10 |
| ATOM | 1175 | CD | GLN | 1035 | 98.983 | 56.413 | 49.112 | 1.00 | 43.12 |
| ATOM | 1176 | OE1 | GLN | 1035 | 98.743 | 56.056 | 50.271 | 1.00 | 44.84 |
| ATOM | 1177 | NE2 | GLN | 1035 | 99.238 | 57.678 | 48.790 | 1.00 | 45.69 |
| ATOM | 1178 | C | GLN | 1035 | 98.234 | 53.851 | 45.655 | 1.00 | 27.03 |
| ATOM | 1179 | O | GLN | 1035 | 98.750 | 52.741 | 45.726 | 1.00 | 29.15 |
| ATOM | 1180 | N | THR | 1036 | 98.582 | 54.745 | 44.738 | 1.00 | 26.03 |
| ATOM | 1181 | CA | THR | 1036 | 99.584 | 54.437 | 43.735 | 1.00 | 25.05 |
| ATOM | 1182 | CB | THR | 1036 | 99.094 | 54.813 | 42.363 | 1.00 | 24.90 |
| ATOM | 1183 | OG1 | THR | 1036 | 98.718 | 56.192 | 42.375 | 1.00 | 25.74 |
| ATOM | 1184 | CG2 | THR | 1036 | 97.901 | 53.967 | 41.988 | 1.00 | 23.85 |
| ATOM | 1185 | C | THR | 1036 | 100.911 | 55.131 | 43.976 | 1.00 | 26.04 |
| ATOM | 1186 | O | THR | 1036 | 101.933 | 54.712 | 43.427 | 1.00 | 27.67 |
| ATOM | 1187 | N | ARG | 1037 | 100.895 | 56.232 | 44.719 | 1.00 | 25.73 |
| ATOM | 1188 | CA | ARG | 1037 | 102.137 | 56.928 | 45.023 | 1.00 | 25.76 |
| ATOM | 1189 | CB | ARG | 1037 | 102.596 | 57.805 | 43.873 | 1.00 | 25.31 |
| ATOM | 1190 | CG | ARG | 1037 | 101.623 | 58.844 | 43.446 | 1.00 | 27.06 |
| ATOM | 1191 | CD | ARG | 1037 | 102.326 | 59.847 | 42.575 | 1.00 | 27.29 |
| ATOM | 1192 | NE | ARG | 1037 | 103.303 | 59.215 | 41.696 | 1.00 | 25.59 |
| ATOM | 1193 | CZ | ARG | 1037 | 103.077 | 58.933 | 40.421 | 1.00 | 27.51 |
| ATOM | 1194 | NH1 | ARG | 1037 | 101.893 | 59.223 | 39.877 | 1.00 | 27.27 |
| ATOM | 1195 | NH2 | ARG | 1037 | 104.048 | 58.402 | 39.685 | 1.00 | 23.57 |
| ATOM | 1196 | C | ARG | 1037 | 102.088 | 57.727 | 46.303 | 1.00 | 26.18 |
| ATOM | 1197 | O | ARG | 1037 | 101.011 | 58.021 | 46.813 | 1.00 | 26.32 |
| ATOM | 1198 | N | GLY | 1038 | 103.266 | 58.059 | 46.823 | 1.00 | 26.76 |
| ATOM | 1199 | CA | GLY | 1038 | 103.348 | 58.806 | 48.064 | 1.00 | 28.78 |
| ATOM | 1200 | C | GLY | 1038 | 103.715 | 60.268 | 47.914 | 1.00 | 29.65 |

FIGURE 3 (CONT.)

| ATOM | 1201 | O | GLY | 1038 | 103.913 | 60.769 | 46.805 | 1.00 | 30.89 |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 1202 | N | LEU | 1039 | 103.865 | 60.929 | 49.054 | 1.00 | 29.52 |
| ATOM | 1203 | CA | LEU | 1039 | 104.199 | 62.346 | 49.135 | 1.00 | 30.82 |
| ATOM | 1204 | CB | LEU | 1039 | 104.550 | 62.670 | 50.582 | 1.00 | 34.94 |
| ATOM | 1205 | CG | LEU | 1039 | 104.045 | 63.977 | 51.184 | 1.00 | 39.14 |
| ATOM | 1206 | CD1 | LEU | 1039 | 103.634 | 63.744 | 52.648 | 1.00 | 41.57 |
| ATOM | 1207 | CD2 | LEU | 1039 | 105.127 | 65.038 | 51.079 | 1.00 | 41.24 |
| ATOM | 1208 | C | LEU | 1039 | 105.342 | 62.782 | 48.214 | 1.00 | 30.11 |
| ATOM | 1209 | O | LEU | 1039 | 105.161 | 63.647 | 47.354 | 1.00 | 29.71 |
| ATOM | 1210 | N | LEU | 1040 | 106.495 | 62.136 | 48.358 | 1.00 | 28.91 |
| ATOM | 1211 | CA | LEU | 1040 | 107.676 | 62.463 | 47.568 | 1.00 | 27.58 |
| ATOM | 1212 | CB | LEU | 1040 | 108.878 | 61.685 | 48.098 | 1.00 | 28.69 |
| ATOM | 1213 | CG | LEU | 1040 | 110.213 | 62.413 | 47.959 | 1.00 | 30.89 |
| ATOM | 1214 | CD1 | LEU | 1040 | 110.195 | 63.632 | 48.870 | 1.00 | 32.42 |
| ATOM | 1215 | CD2 | LEU | 1040 | 111.358 | 61.492 | 48.325 | 1.00 | 30.06 |
| ATOM | 1216 | C | LEU | 1040 | 107.524 | 62.221 | 46.061 | 1.00 | 26.74 |
| ATOM | 1217 | O | LEU | 1040 | 107.899 | 63.068 | 45.242 | 1.00 | 28.09 |
| ATOM | 1218 | N | GLY | 1041 | 106.994 | 61.062 | 45.695 | 1.00 | 24.50 |
| ATOM | 1219 | CA | GLY | 1041 | 106.813 | 60.750 | 44.291 | 1.00 | 23.28 |
| ATOM | 1220 | C | GLY | 1041 | 105.798 | 61.679 | 43.667 | 1.00 | 23.92 |
| ATOM | 1221 | O | GLY | 1041 | 105.922 | 62.054 | 42.498 | 1.00 | 22.23 |
| ATOM | 1222 | N | CYS | 1042 | 104.788 | 62.050 | 44.449 | 1.00 | 23.15 |
| ATOM | 1223 | CA | CYS | 1042 | 103.751 | 62.955 | 43.981 | 1.00 | 23.53 |
| ATOM | 1224 | CB | CYS | 1042 | 102.688 | 63.138 | 45.060 | 1.00 | 25.84 |
| ATOM | 1225 | SG | CYS | 1042 | 101.422 | 64.376 | 44.680 | 1.00 | 27.73 |
| ATOM | 1226 | C | CYS | 1042 | 104.398 | 64.289 | 43.627 | 1.00 | 23.74 |
| ATOM | 1227 | O | CYS | 1042 | 104.253 | 64.771 | 42.507 | 1.00 | 25.62 |
| ATOM | 1228 | N | ILE | 1043 | 105.183 | 64.835 | 44.555 | 1.00 | 23.35 |
| ATOM | 1229 | CA | ILE | 1043 | 105.878 | 66.110 | 44.350 | 1.00 | 20.45 |
| ATOM | 1230 | CB | ILE | 1043 | 106.720 | 66.484 | 45.593 | 1.00 | 20.32 |
| ATOM | 1231 | CG2 | ILE | 1043 | 107.437 | 67.810 | 45.373 | 1.00 | 20.94 |
| ATOM | 1232 | CG1 | ILE | 1043 | 105.815 | 66.571 | 46.831 | 1.00 | 18.68 |
| ATOM | 1233 | CD1 | ILE | 1043 | 106.557 | 66.802 | 48.145 | 1.00 | 18.48 |
| ATOM | 1234 | C | ILE | 1043 | 106.765 | 66.086 | 43.103 | 1.00 | 20.27 |
| ATOM | 1235 | O | ILE | 1043 | 106.645 | 66.952 | 42.242 | 1.00 | 23.53 |
| ATOM | 1236 | N | ILE | 1044 | 107.622 | 65.077 | 42.981 | 1.00 | 20.30 |
| ATOM | 1237 | CA | ILE | 1044 | 108.502 | 64.965 | 41.817 | 1.00 | 19.23 |
| ATOM | 1238 | CB | ILE | 1044 | 109.370 | 63.680 | 41.878 | 1.00 | 18.89 |
| ATOM | 1239 | CG2 | ILE | 1044 | 110.205 | 63.532 | 40.616 | 1.00 | 15.12 |
| ATOM | 1240 | CG1 | ILE | 1044 | 110.276 | 63.720 | 43.108 | 1.00 | 17.13 |
| ATOM | 1241 | CD1 | ILE | 1044 | 110.979 | 62.422 | 43.383 | 1.00 | 19.28 |
| ATOM | 1242 | C | ILE | 1044 | 107.673 | 64.942 | 40.541 | 1.00 | 20.68 |
| ATOM | 1243 | O | ILE | 1044 | 107.921 | 65.721 | 39.621 | 1.00 | 21.41 |
| ATOM | 1244 | N | THR | 1045 | 106.647 | 64.094 | 40.513 | 1.00 | 23.02 |
| ATOM | 1245 | CA | THR | 1045 | 105.779 | 63.968 | 39.340 | 1.00 | 22.82 |
| ATOM | 1246 | CB | THR | 1045 | 104.744 | 62.848 | 39.515 | 1.00 | 22.67 |
| ATOM | 1247 | OG1 | THR | 1045 | 105.415 | 61.631 | 39.874 | 1.00 | 23.02 |
| ATOM | 1248 | CG2 | THR | 1045 | 103.985 | 62.630 | 38.219 | 1.00 | 21.21 |
| ATOM | 1249 | C | THR | 1045 | 105.044 | 65.260 | 39.055 | 1.00 | 23.69 |
| ATOM | 1250 | O | THR | 1045 | 104.773 | 65.583 | 37.903 | 1.00 | 26.48 |
| ATOM | 1251 | N | SER | 1046 | 104.750 | 66.013 | 40.106 | 1.00 | 23.58 |

50/60

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1252 | CA | SER | 1046 | 104.043 | 67.273 | 39.960 | 1.00 | 24.58 |
| ATOM | 1253 | CB | SER | 1046 | 103.691 | 67.852 | 41.331 | 1.00 | 25.34 |
| ATOM | 1254 | OG | SER | 1046 | 102.926 | 69.034 | 41.195 | 1.00 | 26.40 |
| ATOM | 1255 | C | SER | 1046 | 104.895 | 68.264 | 39.205 | 1.00 | 25.37 |
| ATOM | 1256 | O | SER | 1046 | 104.397 | 69.000 | 38.355 | 1.00 | 25.66 |
| ATOM | 1257 | N | LEU | 1047 | 106.183 | 68.281 | 39.521 | 1.00 | 25.73 |
| ATOM | 1258 | CA | LEU | 1047 | 107.094 | 69.204 | 38.873 | 1.00 | 26.65 |
| ATOM | 1259 | CB | LEU | 1047 | 108.316 | 69.450 | 39.759 | 1.00 | 26.72 |
| ATOM | 1260 | CG | LEU | 1047 | 107.985 | 69.811 | 41.217 | 1.00 | 26.90 |
| ATOM | 1261 | CD1 | LEU | 1047 | 109.237 | 70.265 | 41.944 | 1.00 | 25.51 |
| ATOM | 1262 | CD2 | LEU | 1047 | 106.920 | 70.890 | 41.284 | 1.00 | 26.82 |
| ATOM | 1263 | C | LEU | 1047 | 107.494 | 68.762 | 37.466 | 1.00 | 27.72 |
| ATOM | 1264 | O | LEU | 1047 | 107.461 | 69.561 | 36.535 | 1.00 | 29.56 |
| ATOM | 1265 | N | THR | 1048 | 107.806 | 67.483 | 37.288 | 1.00 | 28.48 |
| ATOM | 1266 | CA | THR | 1048 | 108.203 | 66.992 | 35.968 | 1.00 | 27.84 |
| ATOM | 1267 | CB | THR | 1048 | 108.815 | 65.591 | 36.046 | 1.00 | 26.24 |
| ATOM | 1268 | OG1 | THR | 1048 | 107.818 | 64.666 | 36.495 | 1.00 | 28.13 |
| ATOM | 1269 | CG2 | THR | 1048 | 110.002 | 65.580 | 37.001 | 1.00 | 23.61 |
| ATOM | 1270 | C | THR | 1048 | 107.022 | 66.936 | 35.008 | 1.00 | 28.29 |
| ATOM | 1271 | O | THR | 1048 | 107.167 | 67.168 | 33.802 | 1.00 | 28.96 |
| ATOM | 1272 | N | GLY | 1049 | 105.860 | 66.592 | 35.553 | 1.00 | 29.55 |
| ATOM | 1273 | CA | GLY | 1049 | 104.652 | 66.490 | 34.759 | 1.00 | 28.26 |
| ATOM | 1274 | C | GLY | 1049 | 104.582 | 65.197 | 33.975 | 1.00 | 28.82 |
| ATOM | 1275 | O | GLY | 1049 | 103.734 | 65.051 | 33.096 | 1.00 | 27.69 |
| ATOM | 1276 | N | ARG | 1050 | 105.447 | 64.242 | 34.304 | 1.00 | 29.15 |
| ATOM | 1277 | CA | ARG | 1050 | 105.464 | 62.968 | 33.595 | 1.00 | 30.31 |
| ATOM | 1278 | CB | ARG | 1050 | 106.852 | 62.709 | 33.002 | 1.00 | 32.91 |
| ATOM | 1279 | CG | ARG | 1050 | 106.864 | 61.866 | 31.728 | 1.00 | 39.62 |
| ATOM | 1280 | CD | ARG | 1050 | 108.295 | 61.494 | 31.320 | 1.00 | 46.14 |
| ATOM | 1281 | NE | ARG | 1050 | 108.577 | 60.054 | 31.442 | 1.00 | 52.84 |
| ATOM | 1282 | CZ | ARG | 1050 | 109.518 | 59.516 | 32.227 | 1.00 | 55.48 |
| ATOM | 1283 | NH1 | ARG | 1050 | 110.290 | 60.283 | 32.990 | 1.00 | 58.74 |
| ATOM | 1284 | NH2 | ARG | 1050 | 109.730 | 58.204 | 32.208 | 1.00 | 55.47 |
| ATOM | 1285 | C | ARG | 1050 | 105.085 | 61.875 | 34.586 | 1.00 | 29.07 |
| ATOM | 1286 | O | ARG | 1050 | 105.691 | 61.751 | 35.643 | 1.00 | 29.25 |
| ATOM | 1287 | N | ASP | 1051 | 104.040 | 61.123 | 34.267 | 1.00 | 28.54 |
| ATOM | 1288 | CA | ASP | 1051 | 103.572 | 60.054 | 35.133 | 1.00 | 27.21 |
| ATOM | 1289 | CB | ASP | 1051 | 102.214 | 60.412 | 35.729 | 1.00 | 28.72 |
| ATOM | 1290 | CG | ASP | 1051 | 101.694 | 59.357 | 36.684 | 1.00 | 27.51 |
| ATOM | 1291 | OD1 | ASP | 1051 | 102.495 | 58.544 | 37.189 | 1.00 | 29.23 |
| ATOM | 1292 | OD2 | ASP | 1051 | 100.478 | 59.354 | 36.941 | 1.00 | 27.37 |
| ATOM | 1293 | C | ASP | 1051 | 103.446 | 58.790 | 34.320 | 1.00 | 28.42 |
| ATOM | 1294 | O | ASP | 1051 | 102.531 | 58.658 | 33.513 | 1.00 | 29.82 |
| ATOM | 1295 | N | LYS | 1052 | 104.359 | 57.857 | 34.551 | 1.00 | 29.39 |
| ATOM | 1296 | CA | LYS | 1052 | 104.369 | 56.596 | 33.830 | 1.00 | 30.29 |
| ATOM | 1297 | CB | LYS | 1052 | 105.808 | 56.117 | 33.647 | 1.00 | 32.22 |
| ATOM | 1298 | CG | LYS | 1052 | 106.598 | 56.878 | 32.577 | 1.00 | 35.28 |
| ATOM | 1299 | CD | LYS | 1052 | 106.059 | 56.579 | 31.175 | 1.00 | 38.64 |
| ATOM | 1300 | CE | LYS | 1052 | 106.089 | 55.073 | 30.869 | 1.00 | 41.17 |
| ATOM | 1301 | NZ | LYS | 1052 | 105.403 | 54.714 | 29.588 | 1.00 | 42.32 |
| ATOM | 1302 | C | LYS | 1052 | 103.512 | 55.485 | 34.447 | 1.00 | 31.22 |

| ATOM | 1303 | O | LYS | 1052 | 103.356 | 54.424 | 33.841 | 1.00 | 33.64 |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 1304 | N | ASN | 1053 | 102.965 | 55.718 | 35.641 | 1.00 | 29.10 |
| ATOM | 1305 | CA | ASN | 1053 | 102.123 | 54.718 | 36.301 | 1.00 | 26.26 |
| ATOM | 1306 | CB | ASN | 1053 | 101.581 | 55.233 | 37.631 | 1.00 | 25.64 |
| ATOM | 1307 | CG | ASN | 1053 | 102.609 | 55.207 | 38.727 | 1.00 | 23.95 |
| ATOM | 1308 | OD1 | ASN | 1053 | 103.801 | 55.064 | 38.468 | 1.00 | 26.76 |
| ATOM | 1309 | ND2 | ASN | 1053 | 102.161 | 55.363 | 39.963 | 1.00 | 22.69 |
| ATOM | 1310 | C | ASN | 1053 | 100.942 | 54.380 | 35.427 | 1.00 | 26.87 |
| ATOM | 1311 | O | ASN | 1053 | 100.483 | 55.222 | 34.649 | 1.00 | 26.93 |
| ATOM | 1312 | N | ALA | 1054 | 100.457 | 53.147 | 35.545 | 1.00 | 27.34 |
| ATOM | 1313 | CA | ALA | 1054 | 99.301 | 52.713 | 34.766 | 1.00 | 27.38 |
| ATOM | 1314 | CB | ALA | 1054 | 99.275 | 51.196 | 34.623 | 1.00 | 29.92 |
| ATOM | 1315 | C | ALA | 1054 | 98.056 | 53.200 | 35.487 | 1.00 | 26.71 |
| ATOM | 1316 | O | ALA | 1054 | 98.049 | 53.329 | 36.720 | 1.00 | 26.64 |
| ATOM | 1317 | N | VAL | 1055 | 97.009 | 53.474 | 34.716 | 1.00 | 25.91 |
| ATOM | 1318 | CA | VAL | 1055 | 95.761 | 53.978 | 35.269 | 1.00 | 24.92 |
| ATOM | 1319 | CB | VAL | 1055 | 95.262 | 55.216 | 34.476 | 1.00 | 22.35 |
| ATOM | 1320 | CG1 | VAL | 1055 | 93.954 | 55.731 | 35.052 | 1.00 | 22.08 |
| ATOM | 1321 | CG2 | VAL | 1055 | 96.296 | 56.310 | 34.517 | 1.00 | 20.14 |
| ATOM | 1322 | C | VAL | 1055 | 94.681 | 52.908 | 35.257 | 1.00 | 24.94 |
| ATOM | 1323 | O | VAL | 1055 | 94.641 | 52.064 | 34.367 | 1.00 | 24.51 |
| ATOM | 1324 | N | GLU | 1056 | 93.826 | 52.938 | 36.269 | 1.00 | 25.14 |
| ATOM | 1325 | CA | GLU | 1056 | 92.720 | 52.008 | 36.377 | 1.00 | 25.82 |
| ATOM | 1326 | CB | GLU | 1056 | 93.123 | 50.767 | 37.163 | 1.00 | 28.83 |
| ATOM | 1327 | CG | GLU | 1056 | 93.973 | 49.772 | 36.406 | 1.00 | 36.03 |
| ATOM | 1328 | CD | GLU | 1056 | 93.831 | 48.360 | 36.961 | 1.00 | 42.08 |
| ATOM | 1329 | OE1 | GLU | 1056 | 93.640 | 48.210 | 38.191 | 1.00 | 43.57 |
| ATOM | 1330 | OE2 | GLU | 1056 | 93.889 | 47.398 | 36.159 | 1.00 | 46.03 |
| ATOM | 1331 | C | GLU | 1056 | 91.614 | 52.702 | 37.131 | 1.00 | 24.57 |
| ATOM | 1332 | O | GLU | 1056 | 91.856 | 53.700 | 37.810 | 1.00 | 26.39 |
| ATOM | 1333 | N | GLY | 1057 | 90.399 | 52.189 | 37.006 | 1.00 | 22.01 |
| ATOM | 1334 | CA | GLY | 1057 | 89.293 | 52.773 | 37.737 | 1.00 | 20.85 |
| ATOM | 1335 | C | GLY | 1057 | 88.552 | 53.902 | 37.067 | 1.00 | 19.15 |
| ATOM | 1336 | O | GLY | 1057 | 89.013 | 54.476 | 36.079 | 1.00 | 19.49 |
| ATOM | 1337 | N | GLU | 1058 | 87.385 | 54.203 | 37.631 | 1.00 | 19.23 |
| ATOM | 1338 | CA | GLU | 1058 | 86.479 | 55.239 | 37.141 | 1.00 | 16.31 |
| ATOM | 1339 | CB | GLU | 1058 | 85.026 | 54.871 | 37.479 | 1.00 | 15.32 |
| ATOM | 1340 | CG | GLU | 1058 | 84.457 | 53.613 | 36.792 | 1.00 | 15.36 |
| ATOM | 1341 | CD | GLU | 1058 | 85.101 | 52.303 | 37.238 | 1.00 | 18.10 |
| ATOM | 1342 | OE1 | GLU | 1058 | 85.591 | 52.192 | 38.377 | 1.00 | 20.29 |
| ATOM | 1343 | OE2 | GLU | 1058 | 85.118 | 51.359 | 36.434 | 1.00 | 24.06 |
| ATOM | 1344 | C | GLU | 1058 | 86.804 | 56.561 | 37.803 | 1.00 | 15.32 |
| ATOM | 1345 | O | GLU | 1058 | 86.610 | 57.623 | 37.224 | 1.00 | 15.89 |
| ATOM | 1346 | N | VAL | 1059 | 87.292 | 56.485 | 39.034 | 1.00 | 14.97 |
| ATOM | 1347 | CA | VAL | 1059 | 87.629 | 57.661 | 39.818 | 1.00 | 12.63 |
| ATOM | 1348 | CB | VAL | 1059 | 86.813 | 57.684 | 41.136 | 1.00 | 9.72 |
| ATOM | 1349 | CG1 | VAL | 1059 | 86.972 | 59.015 | 41.839 | 1.00 | 10.00 |
| ATOM | 1350 | CG2 | VAL | 1059 | 85.345 | 57.395 | 40.862 | 1.00 | 7.03 |
| ATOM | 1351 | C | VAL | 1059 | 89.121 | 57.661 | 40.156 | 1.00 | 14.78 |
| ATOM | 1352 | O | VAL | 1059 | 89.656 | 56.673 | 40.648 | 1.00 | 15.26 |
| ATOM | 1353 | N | GLN | 1060 | 89.796 | 58.759 | 39.845 | 1.00 | 16.52 |

FIGURE 3 (CONT.)

| ATOM | 1354 | CA  | GLN | 1060 | 91.212  | 58.894 | 40.140 | 1.00 | 16.47 |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 1355 | CB  | GLN | 1060 | 91.936  | 59.556 | 38.967 | 1.00 | 15.66 |
| ATOM | 1356 | CG  | GLN | 1060 | 91.816  | 58.816 | 37.670 | 1.00 | 17.53 |
| ATOM | 1357 | CD  | GLN | 1060 | 92.215  | 57.361 | 37.809 | 1.00 | 20.63 |
| ATOM | 1358 | OE1 | GLN | 1060 | 93.215  | 57.037 | 38.448 | 1.00 | 22.69 |
| ATOM | 1359 | NE2 | GLN | 1060 | 91.424  | 56.474 | 37.229 | 1.00 | 22.24 |
| ATOM | 1360 | C   | GLN | 1060 | 91.367  | 59.775 | 41.372 | 1.00 | 18.64 |
| ATOM | 1361 | O   | GLN | 1060 | 90.702  | 60.801 | 41.496 | 1.00 | 21.76 |
| ATOM | 1362 | N   | ILE | 1061 | 92.175  | 59.345 | 42.326 | 1.00 | 19.32 |
| ATOM | 1363 | CA  | ILE | 1061 | 92.410  | 60.171 | 43.499 | 1.00 | 19.78 |
| ATOM | 1364 | CB  | ILE | 1061 | 92.838  | 59.329 | 44.718 | 1.00 | 18.89 |
| ATOM | 1365 | CG2 | ILE | 1061 | 93.064  | 60.225 | 45.926 | 1.00 | 18.02 |
| ATOM | 1366 | CG1 | ILE | 1061 | 91.759  | 58.289 | 45.033 | 1.00 | 16.75 |
| ATOM | 1367 | CD1 | ILE | 1061 | 92.138  | 57.352 | 46.120 | 1.00 | 14.36 |
| ATOM | 1368 | C   | ILE | 1061 | 93.552  | 61.068 | 43.030 | 1.00 | 21.51 |
| ATOM | 1369 | O   | ILE | 1061 | 94.615  | 60.579 | 42.626 | 1.00 | 22.71 |
| ATOM | 1370 | N   | VAL | 1062 | 93.305  | 62.370 | 42.979 | 1.00 | 21.91 |
| ATOM | 1371 | CA  | VAL | 1062 | 94.321  | 63.294 | 42.515 | 1.00 | 19.92 |
| ATOM | 1372 | CB  | VAL | 1062 | 93.858  | 64.075 | 41.278 | 1.00 | 18.17 |
| ATOM | 1373 | CG1 | VAL | 1062 | 93.500  | 63.117 | 40.166 | 1.00 | 15.34 |
| ATOM | 1374 | CG2 | VAL | 1062 | 92.692  | 64.977 | 41.622 | 1.00 | 15.73 |
| ATOM | 1375 | C   | VAL | 1062 | 94.776  | 64.252 | 43.588 | 1.00 | 21.02 |
| ATOM | 1376 | O   | VAL | 1062 | 94.099  | 64.449 | 44.593 | 1.00 | 22.09 |
| ATOM | 1377 | N   | SER | 1063 | 95.937  | 64.850 | 43.367 | 1.00 | 22.93 |
| ATOM | 1378 | CA  | SER | 1063 | 96.500  | 65.776 | 44.324 | 1.00 | 23.94 |
| ATOM | 1379 | CB  | SER | 1063 | 97.290  | 64.996 | 45.370 | 1.00 | 25.73 |
| ATOM | 1380 | OG  | SER | 1063 | 97.794  | 65.862 | 46.369 | 1.00 | 32.24 |
| ATOM | 1381 | C   | SER | 1063 | 97.413  | 66.795 | 43.673 | 1.00 | 23.42 |
| ATOM | 1382 | O   | SER | 1063 | 97.944  | 66.587 | 42.578 | 1.00 | 20.31 |
| ATOM | 1383 | N   | THR | 1064 | 97.587  | 67.897 | 44.382 | 1.00 | 26.57 |
| ATOM | 1384 | CA  | THR | 1064 | 98.446  | 69.005 | 43.978 | 1.00 | 29.88 |
| ATOM | 1385 | CB  | THR | 1064 | 97.629  | 70.305 | 43.763 | 1.00 | 27.45 |
| ATOM | 1386 | OG1 | THR | 1064 | 97.036  | 70.707 | 45.004 | 1.00 | 25.21 |
| ATOM | 1387 | CG2 | THR | 1064 | 96.523  | 70.086 | 42.751 | 1.00 | 26.09 |
| ATOM | 1388 | C   | THR | 1064 | 99.358  | 69.202 | 45.194 | 1.00 | 32.85 |
| ATOM | 1389 | O   | THR | 1064 | 99.408  | 68.350 | 46.086 | 1.00 | 34.87 |
| ATOM | 1390 | N   | ALA | 1065 | 100.055 | 70.326 | 45.252 | 1.00 | 35.39 |
| ATOM | 1391 | CA  | ALA | 1065 | 100.924 | 70.604 | 46.388 | 1.00 | 35.88 |
| ATOM | 1392 | CB  | ALA | 1065 | 101.866 | 71.747 | 46.051 | 1.00 | 37.88 |
| ATOM | 1393 | C   | ALA | 1065 | 100.052 | 70.978 | 47.578 | 1.00 | 35.60 |
| ATOM | 1394 | O   | ALA | 1065 | 100.275 | 70.537 | 48.698 | 1.00 | 35.43 |
| ATOM | 1395 | N   | THR | 1066 | 99.028  | 71.772 | 47.307 | 1.00 | 36.74 |
| ATOM | 1396 | CA  | THR | 1066 | 98.119  | 72.240 | 48.339 | 1.00 | 37.72 |
| ATOM | 1397 | CB  | THR | 1066 | 97.434  | 73.583 | 47.895 | 1.00 | 39.54 |
| ATOM | 1398 | OG1 | THR | 1066 | 96.431  | 73.973 | 48.844 | 1.00 | 41.76 |
| ATOM | 1399 | CG2 | THR | 1066 | 96.792  | 73.444 | 46.514 | 1.00 | 40.92 |
| ATOM | 1400 | C   | THR | 1066 | 97.043  | 71.261 | 48.808 | 1.00 | 36.34 |
| ATOM | 1401 | O   | THR | 1066 | 96.641  | 71.307 | 49.975 | 1.00 | 36.42 |
| ATOM | 1402 | N   | GLN | 1067 | 96.608  | 70.340 | 47.952 | 1.00 | 34.64 |
| ATOM | 1403 | CA  | GLN | 1067 | 95.517  | 69.461 | 48.367 | 1.00 | 34.70 |
| ATOM | 1404 | CB  | GLN | 1067 | 91.235  | 70.290 | 48.381 | 1.00 | 36.42 |

| ATOM | 1405 | CG | GLN | 1067 | 93.980 | 70.953 | 47.033 | 1.00 | 40.18 |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1406 | CD | GLN | 1067 | 92.844 | 71.952 | 47.052 | 1.00 | 42.84 |
| ATOM | 1407 | OE1 | GLN | 1067 | 91.783 | 71.704 | 47.632 | 1.00 | 44.48 |
| ATOM | 1408 | NE2 | GLN | 1067 | 93.048 | 73.080 | 46.383 | 1.00 | 45.42 |
| ATOM | 1409 | C | GLN | 1067 | 95.263 | 68.210 | 47.536 | 1.00 | 32.18 |
| ATOM | 1410 | O | GLN | 1067 | 95.813 | 68.051 | 46.449 | 1.00 | 32.90 |
| ATOM | 1411 | N | THR | 1068 | 94.379 | 67.357 | 48.054 | 1.00 | 29.91 |
| ATOM | 1412 | CA | THR | 1068 | 93.972 | 66.108 | 47.413 | 1.00 | 27.99 |
| ATOM | 1413 | CB | THR | 1068 | 94.296 | 64.860 | 48.291 | 1.00 | 28.36 |
| ATOM | 1414 | OG1 | THR | 1068 | 95.710 | 64.751 | 48.488 | 1.00 | 30.82 |
| ATOM | 1415 | CG2 | THR | 1068 | 93.788 | 63.581 | 47.636 | 1.00 | 26.64 |
| ATOM | 1416 | C | THR | 1068 | 92.460 | 66.158 | 47.248 | 1.00 | 25.47 |
| ATOM | 1417 | O | THR | 1068 | 91.745 | 66.644 | 48.126 | 1.00 | 25.64 |
| ATOM | 1418 | N | PHE | 1069 | 91.988 | 65.670 | 46.112 | 1.00 | 23.13 |
| ATOM | 1419 | CA | PHE | 1069 | 90.565 | 65.621 | 45.801 | 1.00 | 20.30 |
| ATOM | 1420 | CB | PHE | 1069 | 90.060 | 66.960 | 45.222 | 1.00 | 19.44 |
| ATOM | 1421 | CG | PHE | 1069 | 91.012 | 67.618 | 44.258 | 1.00 | 18.91 |
| ATOM | 1422 | CD1 | PHE | 1069 | 90.765 | 67.593 | 42.890 | 1.00 | 16.69 |
| ATOM | 1423 | CD2 | PHE | 1069 | 92.174 | 68.237 | 44.720 | 1.00 | 16.99 |
| ATOM | 1424 | CE1 | PHE | 1069 | 91.663 | 68.165 | 41.998 | 1.00 | 17.12 |
| ATOM | 1425 | CE2 | PHE | 1069 | 93.075 | 68.811 | 43.838 | 1.00 | 15.95 |
| ATOM | 1426 | CZ | PHE | 1069 | 92.822 | 68.775 | 42.475 | 1.00 | 17.86 |
| ATOM | 1427 | C | PHE | 1069 | 90.340 | 64.454 | 44.840 | 1.00 | 19.50 |
| ATOM | 1428 | O | PHE | 1069 | 91.216 | 63.590 | 44.687 | 1.00 | 18.25 |
| ATOM | 1429 | N | LEU | 1070 | 89.171 | 64.402 | 44.216 | 1.00 | 17.14 |
| ATOM | 1430 | CA | LEU | 1070 | 88.872 | 63.320 | 43.297 | 1.00 | 16.12 |
| ATOM | 1431 | CB | LEU | 1070 | 87.699 | 62.499 | 43.806 | 1.00 | 15.63 |
| ATOM | 1432 | CG | LEU | 1070 | 87.908 | 61.837 | 45.157 | 1.00 | 13.76 |
| ATOM | 1433 | CD1 | LEU | 1070 | 86.650 | 61.104 | 45.531 | 1.00 | 16.70 |
| ATOM | 1434 | CD2 | LEU | 1070 | 89.072 | 60.890 | 45.082 | 1.00 | 15.02 |
| ATOM | 1435 | C | LEU | 1070 | 88.545 | 63.848 | 41.926 | 1.00 | 16.35 |
| ATOM | 1436 | O | LEU | 1070 | 88.181 | 65.011 | 41.774 | 1.00 | 18.69 |
| ATOM | 1437 | N | ALA | 1071 | 88.703 | 62.989 | 40.929 | 1.00 | 15.91 |
| ATOM | 1438 | CA | ALA | 1071 | 88.417 | 63.323 | 39.544 | 1.00 | 15.63 |
| ATOM | 1439 | CB | ALA | 1071 | 89.701 | 63.547 | 38.773 | 1.00 | 14.74 |
| ATOM | 1440 | C | ALA | 1071 | 87.717 | 62.086 | 39.050 | 1.00 | 16.11 |
| ATOM | 1441 | O | ALA | 1071 | 88.194 | 60.981 | 39.278 | 1.00 | 16.97 |
| ATOM | 1442 | N | THR | 1072 | 86.572 | 62.273 | 38.410 | 1.00 | 17.64 |
| ATOM | 1443 | CA | THR | 1072 | 85.764 | 61.171 | 37.914 | 1.00 | 15.73 |
| ATOM | 1444 | CB | THR | 1072 | 84.329 | 61.312 | 38.416 | 1.00 | 15.97 |
| ATOM | 1445 | OG1 | THR | 1072 | 84.344 | 61.551 | 39.827 | 1.00 | 18.30 |
| ATOM | 1446 | CG2 | THR | 1072 | 83.539 | 60.052 | 38.134 | 1.00 | 18.15 |
| ATOM | 1447 | C | THR | 1072 | 85.725 | 61.166 | 36.405 | 1.00 | 14.68 |
| ATOM | 1448 | O | THR | 1072 | 85.511 | 62.197 | 35.786 | 1.00 | 16.38 |
| ATOM | 1449 | N | CYS | 1073 | 85.890 | 59.998 | 35.808 | 1.00 | 14.37 |
| ATOM | 1450 | CA | CYS | 1073 | 85.856 | 59.895 | 34.364 | 1.00 | 15.72 |
| ATOM | 1451 | CB | CYS | 1073 | 86.814 | 58.807 | 33.889 | 1.00 | 17.69 |
| ATOM | 1452 | SG | CYS | 1073 | 88.536 | 59.069 | 34.384 | 1.00 | 23.22 |
| ATOM | 1453 | C | CYS | 1073 | 84.450 | 59.591 | 33.878 | 1.00 | 16.21 |
| ATOM | 1454 | O | CYS | 1073 | 83.850 | 58.601 | 34.286 | 1.00 | 15.04 |
| ATOM | 1455 | N | ILE | 1074 | 83.907 | 60.472 | 33.044 | 1.00 | 17.51 |

FIGURE 3 (CONT.)

| ATOM | 1456 | CA | ILE | 1074 | 82.578 | 60.294 | 32.475 | 1.00 | 20.31 |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 1457 | CB | ILE | 1074 | 81.560 | 61.315 | 33.050 | 1.00 | 20.77 |
| ATOM | 1458 | CG2 | ILE | 1074 | 80.171 | 61.053 | 32.472 | 1.00 | 20.99 |
| ATOM | 1459 | CG1 | ILE | 1074 | 81.509 | 61.221 | 34.580 | 1.00 | 19.74 |
| ATOM | 1460 | CD1 | ILE | 1074 | 80.686 | 62.297 | 35.259 | 1.00 | 16.17 |
| ATOM | 1461 | C | ILE | 1074 | 82.716 | 60.504 | 30.963 | 1.00 | 24.53 |
| ATOM | 1462 | O | ILE | 1074 | 83.299 | 61.493 | 30.521 | 1.00 | 28.24 |
| ATOM | 1463 | N | ASN | 1075 | 82.236 | 59.543 | 30.176 | 1.00 | 27.13 |
| ATOM | 1464 | CA | ASN | 1075 | 82.297 | 59.601 | 28.708 | 1.00 | 25.19 |
| ATOM | 1465 | CB | ASN | 1075 | 81.193 | 60.502 | 28.146 | 1.00 | 24.15 |
| ATOM | 1466 | CG | ASN | 1075 | 79.836 | 59.845 | 28.180 | 1.00 | 20.59 |
| ATOM | 1467 | OD1 | ASN | 1075 | 79.635 | 58.844 | 28.858 | 1.00 | 22.02 |
| ATOM | 1468 | ND2 | ASN | 1075 | 78.894 | 60.406 | 27.453 | 1.00 | 23.38 |
| ATOM | 1469 | C | ASN | 1075 | 83.642 | 59.983 | 28.092 | 1.00 | 26.07 |
| ATOM | 1470 | O | ASN | 1075 | 83.707 | 60.798 | 27.164 | 1.00 | 29.28 |
| ATOM | 1471 | N | GLY | 1076 | 84.718 | 59.394 | 28.602 | 1.00 | 26.05 |
| ATOM | 1472 | CA | GLY | 1076 | 86.040 | 59.670 | 28.059 | 1.00 | 23.82 |
| ATOM | 1473 | C | GLY | 1076 | 86.737 | 60.935 | 28.512 | 1.00 | 22.44 |
| ATOM | 1474 | O | GLY | 1076 | 87.779 | 61.292 | 27.959 | 1.00 | 23.12 |
| ATOM | 1475 | N | VAL | 1077 | 86.202 | 61.595 | 29.534 | 1.00 | 22.15 |
| ATOM | 1476 | CA | VAL | 1077 | 86.799 | 62.820 | 30.048 | 1.00 | 21.41 |
| ATOM | 1477 | CB | VAL | 1077 | 85.933 | 64.056 | 29.706 | 1.00 | 22.29 |
| ATOM | 1478 | CG1 | VAL | 1077 | 86.555 | 65.329 | 30.281 | 1.00 | 22.38 |
| ATOM | 1479 | CG2 | VAL | 1077 | 85.767 | 64.180 | 28.200 | 1.00 | 22.13 |
| ATOM | 1480 | C | VAL | 1077 | 86.950 | 62.729 | 31.558 | 1.00 | 20.92 |
| ATOM | 1481 | O | VAL | 1077 | 86.036 | 62.291 | 32.256 | 1.00 | 22.56 |
| ATOM | 1482 | N | CYS | 1078 | 88.120 | 63.112 | 32.053 | 1.00 | 19.00 |
| ATOM | 1483 | CA | CYS | 1078 | 88.399 | 63.090 | 33.482 | 1.00 | 18.18 |
| ATOM | 1484 | CB | CYS | 1078 | 89.886 | 62.832 | 33.736 | 1.00 | 17.52 |
| ATOM | 1485 | SG | CYS | 1078 | 90.338 | 62.568 | 35.461 | 1.00 | 16.09 |
| ATOM | 1486 | C | CYS | 1078 | 88.008 | 64.441 | 34.045 | 1.00 | 17.95 |
| ATOM | 1487 | O | CYS | 1078 | 88.768 | 65.402 | 33.962 | 1.00 | 21.44 |
| ATOM | 1488 | N | TRP | 1079 | 86.802 | 64.513 | 34.589 | 1.00 | 18.33 |
| ATOM | 1489 | CA | TRP | 1079 | 86.267 | 65.737 | 35.164 | 1.00 | 14.96 |
| ATOM | 1490 | CB | TRP | 1079 | 84.744 | 65.736 | 35.066 | 1.00 | 15.12 |
| ATOM | 1491 | CG | TRP | 1079 | 84.213 | 65.817 | 33.677 | 1.00 | 17.41 |
| ATOM | 1492 | CD2 | TRP | 1079 | 84.023 | 67.007 | 32.903 | 1.00 | 18.04 |
| ATOM | 1493 | CE2 | TRP | 1079 | 83.465 | 66.619 | 31.668 | 1.00 | 19.10 |
| ATOM | 1494 | CE3 | TRP | 1079 | 84.268 | 68.369 | 33.137 | 1.00 | 17.65 |
| ATOM | 1495 | CD1 | TRP | 1079 | 83.780 | 64.781 | 32.904 | 1.00 | 16.78 |
| ATOM | 1496 | NE1 | TRP | 1079 | 83.325 | 65.254 | 31.693 | 1.00 | 19.80 |
| ATOM | 1497 | CZ2 | TRP | 1079 | 83.146 | 67.545 | 30.664 | 1.00 | 19.19 |
| ATOM | 1498 | CZ3 | TRP | 1079 | 83.949 | 69.291 | 32.139 | 1.00 | 15.70 |
| ATOM | 1499 | CH2 | TRP | 1079 | 83.395 | 68.873 | 30.921 | 1.00 | 16.14 |
| ATOM | 1500 | C | TRP | 1079 | 86.631 | 65.895 | 36.619 | 1.00 | 15.06 |
| ATOM | 1501 | O | TRP | 1079 | 86.701 | 64.926 | 37.363 | 1.00 | 14.95 |
| ATOM | 1502 | N | THR | 1080 | 86.851 | 67.129 | 37.034 | 1.00 | 17.34 |
| ATOM | 1503 | CA | THR | 1080 | 87.148 | 67.390 | 38.421 | 1.00 | 19.67 |
| ATOM | 1504 | CB | THR | 1080 | 88.636 | 67.201 | 38.762 | 1.00 | 19.66 |
| ATOM | 1505 | OG1 | THR | 1080 | 88.794 | 67.207 | 40.187 | 1.00 | 18.69 |
| ATOM | 1506 | CG2 | THR | 1080 | 89.475 | 68.299 | 38.162 | 1.00 | 21.67 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1507 | C | THR | 1080 | 86.663 | 68.781 | 38.780 | 1.00 | 21.24 |
| ATOM | 1508 | O | THR | 1080 | 86.113 | 69.499 | 37.938 | 1.00 | 20.94 |
| ATOM | 1509 | N | VAL | 1081 | 86.867 | 69.141 | 40.039 | 1.00 | 23.41 |
| ATOM | 1510 | CA | VAL | 1081 | 86.444 | 70.417 | 40.588 | 1.00 | 23.97 |
| ATOM | 1511 | CB | VAL | 1081 | 86.053 | 70.200 | 42.076 | 1.00 | 22.41 |
| ATOM | 1512 | CG1 | VAL | 1081 | 87.258 | 70.300 | 42.987 | 1.00 | 21.40 |
| ATOM | 1513 | CG2 | VAL | 1081 | 84.918 | 71.094 | 42.474 | 1.00 | 23.79 |
| ATOM | 1514 | C | VAL | 1081 | 87.519 | 71.520 | 40.384 | 1.00 | 25.41 |
| ATOM | 1515 | O | VAL | 1081 | 88.715 | 71.316 | 40.632 | 1.00 | 24.93 |
| ATOM | 1516 | N | TYR | 1082 | 87.093 | 72.683 | 39.903 | 1.00 | 25.72 |
| ATOM | 1517 | CA | TYR | 1082 | 88.016 | 73.785 | 39.643 | 1.00 | 25.46 |
| ATOM | 1518 | CB | TYR | 1082 | 87.321 | 74.892 | 38.840 | 1.00 | 26.17 |
| ATOM | 1519 | CG | TYR | 1082 | 88.245 | 76.005 | 38.392 | 1.00 | 26.30 |
| ATOM | 1520 | CD1 | TYR | 1082 | 88.538 | 77.075 | 39.240 | 1.00 | 26.95 |
| ATOM | 1521 | CE1 | TYR | 1082 | 89.411 | 78.092 | 38.852 | 1.00 | 28.63 |
| ATOM | 1522 | CD2 | TYR | 1082 | 88.846 | 75.973 | 37.138 | 1.00 | 26.52 |
| ATOM | 1523 | CE2 | TYR | 1082 | 89.724 | 76.982 | 36.735 | 1.00 | 29.11 |
| ATOM | 1524 | CZ | TYR | 1082 | 90.006 | 78.038 | 37.600 | 1.00 | 30.48 |
| ATOM | 1525 | OH | TYR | 1082 | 90.886 | 79.038 | 37.222 | 1.00 | 31.27 |
| ATOM | 1526 | C | TYR | 1082 | 88.665 | 74.349 | 40.910 | 1.00 | 25.31 |
| ATOM | 1527 | O | TYR | 1082 | 89.793 | 74.845 | 40.863 | 1.00 | 22.94 |
| ATOM | 1528 | N | HIS | 1083 | 87.986 | 74.239 | 42.049 | 1.00 | 24.48 |
| ATOM | 1529 | CA | HIS | 1083 | 88.568 | 74.748 | 43.283 | 1.00 | 25.01 |
| ATOM | 1530 | CB | HIS | 1083 | 87.514 | 74.963 | 44.378 | 1.00 | 23.89 |
| ATOM | 1531 | CG | HIS | 1083 | 86.984 | 73.707 | 44.999 | 1.00 | 27.06 |
| ATOM | 1532 | CD2 | HIS | 1083 | 87.505 | 72.888 | 45.948 | 1.00 | 28.89 |
| ATOM | 1533 | ND1 | HIS | 1083 | 85.723 | 73.216 | 44.727 | 1.00 | 29.27 |
| ATOM | 1534 | CE1 | HIS | 1083 | 85.488 | 72.155 | 45.479 | 1.00 | 28.81 |
| ATOM | 1535 | NE2 | HIS | 1083 | 86.554 | 71.936 | 46.229 | 1.00 | 30.38 |
| ATOM | 1536 | C | HIS | 1083 | 89.701 | 73.853 | 43.766 | 1.00 | 26.93 |
| ATOM | 1537 | O | HIS | 1083 | 90.266 | 74.073 | 44.837 | 1.00 | 29.65 |
| ATOM | 1538 | N | GLY | 1084 | 90.008 | 72.823 | 42.985 | 1.00 | 25.81 |
| ATOM | 1539 | CA | GLY | 1084 | 91.082 | 71.922 | 43.336 | 1.00 | 23.74 |
| ATOM | 1540 | C | GLY | 1084 | 92.153 | 71.987 | 42.266 | 1.00 | 21.87 |
| ATOM | 1541 | O | GLY | 1084 | 93.286 | 72.360 | 42.540 | 1.00 | 22.00 |
| ATOM | 1542 | N | ALA | 1085 | 91.771 | 71.667 | 41.035 | 1.00 | 21.01 |
| ATOM | 1543 | CA | ALA | 1085 | 92.696 | 71.662 | 39.911 | 1.00 | 20.52 |
| ATOM | 1544 | CB | ALA | 1085 | 92.103 | 70.883 | 38.752 | 1.00 | 18.56 |
| ATOM | 1545 | C | ALA | 1085 | 93.143 | 73.034 | 39.436 | 1.00 | 21.49 |
| ATOM | 1546 | O | ALA | 1085 | 94.273 | 73.192 | 39.000 | 1.00 | 23.82 |
| ATOM | 1547 | N | GLY | 1086 | 92.265 | 74.025 | 39.498 | 1.00 | 22.93 |
| ATOM | 1548 | CA | GLY | 1086 | 92.641 | 75.344 | 39.033 | 1.00 | 22.64 |
| ATOM | 1549 | C | GLY | 1086 | 92.791 | 75.264 | 37.526 | 1.00 | 25.01 |
| ATOM | 1550 | O | GLY | 1086 | 91.981 | 74.631 | 36.851 | 1.00 | 25.80 |
| ATOM | 1551 | N | THR | 1087 | 93.830 | 75.876 | 36.984 | 1.00 | 26.41 |
| ATOM | 1552 | CA | THR | 1087 | 94.032 | 75.829 | 35.544 | 1.00 | 29.05 |
| ATOM | 1553 | CB | THR | 1087 | 94.450 | 77.204 | 35.003 | 1.00 | 32.46 |
| ATOM | 1554 | OG1 | THR | 1087 | 95.572 | 77.683 | 35.758 | 1.00 | 34.46 |
| ATOM | 1555 | CG2 | THR | 1087 | 93.292 | 78.209 | 35.086 | 1.00 | 33.93 |
| ATOM | 1556 | C | THR | 1087 | 95.127 | 74.846 | 35.159 | 1.00 | 28.61 |
| ATOM | 1557 | O | THR | 1087 | 95.422 | 74.679 | 33.971 | 1.00 | 30.95 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1558 | N | ARG | 1088 | 95.689 | 74.145 | 36.138 | 1.00 | 27.72 |
| ATOM | 1559 | CA | ARG | 1088 | 96.793 | 73.247 | 35.837 | 1.00 | 26.27 |
| ATOM | 1560 | CB | ARG | 1088 | 97.606 | 72.923 | 37.083 | 1.00 | 25.05 |
| ATOM | 1561 | CG | ARG | 1088 | 96.830 | 72.482 | 38.249 | 1.00 | 22.82 |
| ATOM | 1562 | CD | ARG | 1088 | 97.651 | 72.707 | 39.472 | 1.00 | 22.84 |
| ATOM | 1563 | NE | ARG | 1088 | 96.964 | 73.601 | 40.382 | 1.00 | 26.47 |
| ATOM | 1564 | CZ | ARG | 1088 | 97.386 | 73.875 | 41.607 | 1.00 | 28.75 |
| ATOM | 1565 | NH1 | ARG | 1088 | 98.505 | 73.324 | 42.068 | 1.00 | 31.62 |
| ATOM | 1566 | NH2 | ARG | 1088 | 96.677 | 74.691 | 42.375 | 1.00 | 29.37 |
| ATOM | 1567 | C | ARG | 1088 | 96.577 | 72.014 | 34.993 | 1.00 | 25.66 |
| ATOM | 1568 | O | ARG | 1088 | 95.448 | 71.583 | 34.752 | 1.00 | 28.07 |
| ATOM | 1569 | N | THR | 1089 | 97.694 | 71.509 | 34.487 | 1.00 | 23.84 |
| ATOM | 1570 | CA | THR | 1089 | 97.736 | 70.343 | 33.633 | 1.00 | 23.41 |
| ATOM | 1571 | CB | THR | 1089 | 99.014 | 70.390 | 32.769 | 1.00 | 23.85 |
| ATOM | 1572 | OG1 | THR | 1089 | 100.146 | 70.668 | 33.602 | 1.00 | 24.27 |
| ATOM | 1573 | CG2 | THR | 1089 | 98.916 | 71.474 | 31.715 | 1.00 | 21.97 |
| ATOM | 1574 | C | THR | 1089 | 97.742 | 69.085 | 34.493 | 1.00 | 23.76 |
| ATOM | 1575 | O | THR | 1089 | 97.876 | 69.172 | 35.717 | 1.00 | 24.27 |
| ATOM | 1576 | N | ILE | 1090 | 97.546 | 67.925 | 33.869 | 1.00 | 21.48 |
| ATOM | 1577 | CA | ILE | 1090 | 97.570 | 66.659 | 34.600 | 1.00 | 20.72 |
| ATOM | 1578 | CB | ILE | 1090 | 96.251 | 65.811 | 34.409 | 1.00 | 19.48 |
| ATOM | 1579 | CG2 | ILE | 1090 | 96.115 | 65.296 | 32.977 | 1.00 | 20.97 |
| ATOM | 1580 | CG1 | ILE | 1090 | 96.216 | 64.642 | 35.405 | 1.00 | 19.86 |
| ATOM | 1581 | CD1 | ILE | 1090 | 94.857 | 63.936 | 35.519 | 1.00 | 15.19 |
| ATOM | 1582 | C | ILE | 1090 | 98.803 | 65.896 | 34.135 | 1.00 | 19.55 |
| ATOM | 1583 | O | ILE | 1090 | 99.091 | 65.841 | 32.940 | 1.00 | 17.18 |
| ATOM | 1584 | N | ALA | 1091 | 99.582 | 65.395 | 35.085 | 1.00 | 19.06 |
| ATOM | 1585 | CA | ALA | 1091 | 100.786 | 64.648 | 34.750 | 1.00 | 17.95 |
| ATOM | 1586 | CB | ALA | 1091 | 101.558 | 64.318 | 36.007 | 1.00 | 15.33 |
| ATOM | 1587 | C | ALA | 1091 | 100.378 | 63.374 | 34.036 | 1.00 | 19.98 |
| ATOM | 1588 | O | ALA | 1091 | 99.509 | 62.643 | 34.515 | 1.00 | 22.10 |
| ATOM | 1589 | N | SER | 1092 | 100.978 | 63.116 | 32.882 | 1.00 | 21.44 |
| ATOM | 1590 | CA | SER | 1092 | 100.667 | 61.913 | 32.128 | 1.00 | 24.34 |
| ATOM | 1591 | CB | SER | 1092 | 99.759 | 62.244 | 30.941 | 1.00 | 24.98 |
| ATOM | 1592 | OG | SER | 1092 | 100.517 | 62.642 | 29.817 | 1.00 | 26.24 |
| ATOM | 1593 | C | SER | 1092 | 101.953 | 61.271 | 31.629 | 1.00 | 25.86 |
| ATOM | 1594 | O | SER | 1092 | 103.030 | 61.838 | 31.771 | 1.00 | 27.85 |
| ATOM | 1595 | N | PRO | 1093 | 101.862 | 60.064 | 31.060 | 1.00 | 27.32 |
| ATOM | 1596 | CD | PRO | 1093 | 100.670 | 59.207 | 30.955 | 1.00 | 28.88 |
| ATOM | 1597 | CA | PRO | 1093 | 103.038 | 59.366 | 30.544 | 1.00 | 29.05 |
| ATOM | 1598 | CB | PRO | 1093 | 102.424 | 58.145 | 29.864 | 1.00 | 29.52 |
| ATOM | 1599 | CG | PRO | 1093 | 101.270 | 57.843 | 30.734 | 1.00 | 30.09 |
| ATOM | 1600 | C | PRO | 1093 | 103.807 | 60.199 | 29.532 | 1.00 | 29.67 |
| ATOM | 1601 | O | PRO | 1093 | 105.029 | 60.101 | 29.450 | 1.00 | 31.90 |
| ATOM | 1602 | N | LYS | 1094 | 103.081 | 61.014 | 28.767 | 1.00 | 29.17 |
| ATOM | 1603 | CA | LYS | 1094 | 103.669 | 61.855 | 27.729 | 1.00 | 28.35 |
| ATOM | 1604 | CB | LYS | 1094 | 102.769 | 61.857 | 26.492 | 1.00 | 25.80 |
| ATOM | 1605 | CG | LYS | 1094 | 102.678 | 60.505 | 25.833 | 1.00 | 26.73 |
| ATOM | 1606 | CD | LYS | 1094 | 102.036 | 60.568 | 24.467 | 1.00 | 28.73 |
| ATOM | 1607 | CE | LYS | 1094 | 102.138 | 59.217 | 23.790 | 1.00 | 30.21 |
| ATOM | 1608 | NZ | LYS | 1094 | 101.569 | 59.241 | 22.428 | 1.00 | 31.93 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1609 | C | LYS | 1094 | 103.934 | 63.281 | 28.177 | 1.00 | 29.51 |
| ATOM | 1610 | O | LYS | 1094 | 104.098 | 64.187 | 27.348 | 1.00 | 31.07 |
| ATOM | 1611 | N | GLY | 1095 | 104.021 | 63.471 | 29.487 | 1.00 | 30.06 |
| ATOM | 1612 | CA | GLY | 1095 | 104.261 | 64.794 | 30.035 | 1.00 | 29.06 |
| ATOM | 1613 | C | GLY | 1095 | 102.962 | 65.406 | 30.514 | 1.00 | 27.34 |
| ATOM | 1614 | O | GLY | 1095 | 101.935 | 64.724 | 30.527 | 1.00 | 28.11 |
| ATOM | 1615 | N | PRO | 1096 | 102.973 | 66.668 | 30.959 | 1.00 | 24.82 |
| ATOM | 1616 | CD | PRO | 1096 | 104.071 | 67.640 | 31.038 | 1.00 | 24.20 |
| ATOM | 1617 | CA | PRO | 1096 | 101.720 | 67.258 | 31.419 | 1.00 | 24.35 |
| ATOM | 1618 | CB | PRO | 1096 | 102.163 | 68.611 | 31.970 | 1.00 | 23.18 |
| ATOM | 1619 | CG | PRO | 1096 | 103.321 | 68.948 | 31.117 | 1.00 | 25.11 |
| ATOM | 1620 | C | PRO | 1096 | 100.732 | 67.401 | 30.268 | 1.00 | 24.48 |
| ATOM | 1621 | O | PRO | 1096 | 101.125 | 67.569 | 29.116 | 1.00 | 25.88 |
| ATOM | 1622 | N | VAL | 1097 | 99.450 | 67.270 | 30.582 | 1.00 | 25.45 |
| ATOM | 1623 | CA | VAL | 1097 | 98.393 | 67.386 | 29.595 | 1.00 | 24.09 |
| ATOM | 1624 | CB | VAL | 1097 | 97.598 | 66.077 | 29.520 | 1.00 | 22.86 |
| ATOM | 1625 | CG1 | VAL | 1097 | 96.393 | 66.224 | 28.609 | 1.00 | 21.59 |
| ATOM | 1626 | CG2 | VAL | 1097 | 98.510 | 64.964 | 29.009 | 1.00 | 23.88 |
| ATOM | 1627 | C | VAL | 1097 | 97.495 | 68.563 | 29.973 | 1.00 | 24.81 |
| ATOM | 1628 | O | VAL | 1097 | 97.051 | 68.675 | 31.113 | 1.00 | 25.35 |
| ATOM | 1629 | N | ILE | 1098 | 97.298 | 69.478 | 29.032 | 1.00 | 25.32 |
| ATOM | 1630 | CA | ILE | 1098 | 96.474 | 70.666 | 29.252 | 1.00 | 25.37 |
| ATOM | 1631 | CB | ILE | 1098 | 96.731 | 71.698 | 28.135 | 1.00 | 27.24 |
| ATOM | 1632 | CG2 | ILE | 1098 | 96.029 | 73.015 | 28.447 | 1.00 | 26.41 |
| ATOM | 1633 | CG1 | ILE | 1098 | 98.247 | 71.932 | 28.008 | 1.00 | 30.74 |
| ATOM | 1634 | CD1 | ILE | 1098 | 98.659 | 72.943 | 26.946 | 1.00 | 32.59 |
| ATOM | 1635 | C | ILE | 1098 | 94.986 | 70.313 | 29.331 | 1.00 | 23.54 |
| ATOM | 1636 | O | ILE | 1098 | 94.546 | 69.325 | 28.752 | 1.00 | 24.20 |
| ATOM | 1637 | N | GLN | 1099 | 94.212 | 71.120 | 30.043 | 1.00 | 20.79 |
| ATOM | 1638 | CA | GLN | 1099 | 92.787 | 70.853 | 30.193 | 1.00 | 20.64 |
| ATOM | 1639 | CB | GLN | 1099 | 92.188 | 71.774 | 31.236 | 1.00 | 16.40 |
| ATOM | 1640 | CG | GLN | 1099 | 92.897 | 71.747 | 32.534 | 1.00 | 17.16 |
| ATOM | 1641 | CD | GLN | 1099 | 92.215 | 72.607 | 33.541 | 1.00 | 20.14 |
| ATOM | 1642 | OE1 | GLN | 1099 | 91.129 | 73.118 | 33.286 | 1.00 | 25.87 |
| ATOM | 1643 | NE2 | GLN | 1099 | 92.827 | 72.767 | 34.704 | 1.00 | 21.32 |
| ATOM | 1644 | C | GLN | 1099 | 91.973 | 70.990 | 28.918 | 1.00 | 22.84 |
| ATOM | 1645 | O | GLN | 1099 | 92.217 | 71.882 | 28.109 | 1.00 | 25.86 |
| ATOM | 1646 | N | MET | 1100 | 91.006 | 70.090 | 28.752 | 1.00 | 23.50 |
| ATOM | 1647 | CA | MET | 1100 | 90.099 | 70.094 | 27.606 | 1.00 | 22.12 |
| ATOM | 1648 | CB | MET | 1100 | 89.418 | 68.737 | 27.447 | 1.00 | 20.94 |
| ATOM | 1649 | CG | MET | 1100 | 90.052 | 67.816 | 26.450 | 1.00 | 22.51 |
| ATOM | 1650 | SD | MET | 1100 | 88.916 | 66.522 | 25.981 | 1.00 | 22.15 |
| ATOM | 1651 | CE | MET | 1100 | 88.786 | 65.731 | 27.470 | 1.00 | 23.27 |
| ATOM | 1652 | C | MET | 1100 | 89.002 | 71.124 | 27.819 | 1.00 | 23.05 |
| ATOM | 1653 | O | MET | 1100 | 88.581 | 71.801 | 26.879 | 1.00 | 24.71 |
| ATOM | 1654 | N | TYR | 1101 | 88.495 | 71.180 | 29.047 | 1.00 | 22.24 |
| ATOM | 1655 | CA | TYR | 1101 | 87.424 | 72.098 | 29.402 | 1.00 | 20.19 |
| ATOM | 1656 | CB | TYR | 1101 | 86.103 | 71.340 | 29.561 | 1.00 | 19.75 |
| ATOM | 1657 | CG | TYR | 1101 | 85.809 | 70.388 | 28.431 | 1.00 | 21.76 |
| ATOM | 1658 | CD1 | TYR | 1101 | 86.004 | 69.022 | 28.582 | 1.00 | 20.14 |
| ATOM | 1659 | CE1 | TYR | 1101 | 85.784 | 68.146 | 27.525 | 1.00 | 22.53 |

FIGURE 3 (CONT.)

| ATOM | 1660 | CD2 | TYR | 1101 | 85.383 | 70.859 | 27.195 | 1.00 | 22.07 |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 1661 | CE2 | TYR | 1101 | 85.161 | 69.998 | 26.137 | 1.00 | 21.98 |
| ATOM | 1662 | CZ | TYR | 1101 | 85.363 | 68.642 | 26.304 | 1.00 | 22.76 |
| ATOM | 1663 | OH | TYR | 1101 | 85.130 | 67.781 | 25.254 | 1.00 | 24.74 |
| ATOM | 1664 | C | TYR | 1101 | 87.750 | 72.764 | 30.716 | 1.00 | 21.21 |
| ATOM | 1665 | O | TYR | 1101 | 88.437 | 72.187 | 31.560 | 1.00 | 22.22 |
| ATOM | 1666 | N | THR | 1102 | 87.236 | 73.973 | 30.890 | 1.00 | 23.24 |
| ATOM | 1667 | CA | THR | 1102 | 87.424 | 74.741 | 32.111 | 1.00 | 24.37 |
| ATOM | 1668 | CB | THR | 1102 | 88.640 | 75.681 | 32.013 | 1.00 | 24.53 |
| ATOM | 1669 | OG1 | THR | 1102 | 89.738 | 74.991 | 31.399 | 1.00 | 23.57 |
| ATOM | 1670 | CG2 | THR | 1102 | 89.047 | 76.169 | 33.403 | 1.00 | 22.58 |
| ATOM | 1671 | C | THR | 1102 | 86.175 | 75.597 | 32.244 | 1.00 | 25.86 |
| ATOM | 1672 | O | THR | 1102 | 85.658 | 76.094 | 31.246 | 1.00 | 28.08 |
| ATOM | 1673 | N | ASN | 1103 | 85.668 | 75.740 | 33.460 | 1.00 | 26.20 |
| ATOM | 1674 | CA | ASN | 1103 | 84.480 | 76.547 | 33.700 | 1.00 | 25.78 |
| ATOM | 1675 | CB | ASN | 1103 | 83.213 | 75.752 | 33.372 | 1.00 | 26.82 |
| ATOM | 1676 | CG | ASN | 1103 | 81.947 | 76.585 | 33.511 | 1.00 | 28.67 |
| ATOM | 1677 | OD1 | ASN | 1103 | 81.932 | 77.609 | 34.199 | 1.00 | 30.76 |
| ATOM | 1678 | ND2 | ASN | 1103 | 80.871 | 76.135 | 32.882 | 1.00 | 27.57 |
| ATOM | 1679 | C | ASN | 1103 | 84.480 | 76.995 | 35.156 | 1.00 | 26.25 |
| ATOM | 1680 | O | ASN | 1103 | 83.832 | 76.391 | 36.006 | 1.00 | 27.25 |
| ATOM | 1681 | N | VAL | 1104 | 85.212 | 78.069 | 35.430 | 1.00 | 27.39 |
| ATOM | 1682 | CA | VAL | 1104 | 85.333 | 78.611 | 36.776 | 1.00 | 28.21 |
| ATOM | 1683 | CB | VAL | 1104 | 86.025 | 79.980 | 36.783 | 1.00 | 27.51 |
| ATOM | 1684 | CG1 | VAL | 1104 | 86.316 | 80.397 | 38.205 | 1.00 | 28.55 |
| ATOM | 1685 | CG2 | VAL | 1104 | 87.298 | 79.948 | 35.963 | 1.00 | 28.06 |
| ATOM | 1686 | C | VAL | 1104 | 83.978 | 78.796 | 37.419 | 1.00 | 30.54 |
| ATOM | 1687 | O | VAL | 1104 | 83.803 | 78.517 | 38.604 | 1.00 | 31.53 |
| ATOM | 1688 | N | ASP | 1105 | 83.022 | 79.260 | 36.626 | 1.00 | 33.66 |
| ATOM | 1689 | CA | ASP | 1105 | 81.677 | 79.503 | 37.117 | 1.00 | 36.82 |
| ATOM | 1690 | CB | ASP | 1105 | 80.788 | 80.061 | 36.001 | 1.00 | 41.34 |
| ATOM | 1691 | CG | ASP | 1105 | 81.192 | 81.457 | 35.573 | 1.00 | 45.36 |
| ATOM | 1692 | OD1 | ASP | 1105 | 81.157 | 82.369 | 36.429 | 1.00 | 47.53 |
| ATOM | 1693 | OD2 | ASP | 1105 | 81.543 | 81.636 | 34.382 | 1.00 | 48.54 |
| ATOM | 1694 | C | ASP | 1105 | 81.058 | 78.241 | 37.676 | 1.00 | 36.71 |
| ATOM | 1695 | O | ASP | 1105 | 80.645 | 78.200 | 38.835 | 1.00 | 36.88 |
| ATOM | 1696 | N | GLN | 1106 | 81.011 | 77.203 | 36.851 | 1.00 | 36.71 |
| ATOM | 1697 | CA | GLN | 1106 | 80.417 | 75.940 | 37.266 | 1.00 | 36.44 |
| ATOM | 1698 | CB | GLN | 1106 | 79.895 | 75.194 | 36.042 | 1.00 | 38.58 |
| ATOM | 1699 | CG | GLN | 1106 | 78.821 | 76.012 | 35.312 | 1.00 | 43.02 |
| ATOM | 1700 | CD | GLN | 1106 | 78.192 | 75.305 | 34.120 | 1.00 | 44.86 |
| ATOM | 1701 | OE1 | GLN | 1106 | 77.334 | 75.870 | 33.437 | 1.00 | 44.11 |
| ATOM | 1702 | NE2 | GLN | 1106 | 78.606 | 74.068 | 33.866 | 1.00 | 47.22 |
| ATOM | 1703 | C | GLN | 1106 | 81.342 | 75.077 | 38.122 | 1.00 | 34.06 |
| ATOM | 1704 | O | GLN | 1106 | 80.930 | 74.029 | 38.625 | 1.00 | 33.78 |
| ATOM | 1705 | N | ASP | 1107 | 82.561 | 75.575 | 38.339 | 1.00 | 29.82 |
| ATOM | 1706 | CA | ASP | 1107 | 83.577 | 74.900 | 39.144 | 1.00 | 26.00 |
| ATOM | 1707 | CB | ASP | 1107 | 83.039 | 74.635 | 40.551 | 1.00 | 26.29 |
| ATOM | 1708 | CG | ASP | 1107 | 84.138 | 74.436 | 41.574 | 1.00 | 25.28 |
| ATOM | 1709 | OD1 | ASP | 1107 | 85.287 | 74.822 | 41.303 | 1.00 | 26.49 |
| ATOM | 1710 | OD2 | ASP | 1107 | 83.844 | 73.914 | 42.666 | 1.00 | 25.48 |

FIGURE 3 (CONT.)

| ATOM | 1711 | C | ASP | 1107 | 84.016 | 73.597 | 38.492 | 1.00 | 23.82 |
|------|------|------|------|------|--------|--------|--------|------|-------|
| ATOM | 1712 | O | ASP | 1107 | 84.348 | 72.637 | 39.176 | 1.00 | 23.57 |
| ATOM | 1713 | N | LEU | 1108 | 84.066 | 73.593 | 37.167 | 1.00 | 21.98 |
| ATOM | 1714 | CA | LEU | 1108 | 84.440 | 72.413 | 36.403 | 1.00 | 22.63 |
| ATOM | 1715 | CB | LEU | 1108 | 83.349 | 72.083 | 35.378 | 1.00 | 21.22 |
| ATOM | 1716 | CG | LEU | 1108 | 82.093 | 71.415 | 35.928 | 1.00 | 21.50 |
| ATOM | 1717 | CD1 | LEU | 1108 | 81.053 | 71.249 | 34.840 | 1.00 | 21.03 |
| ATOM | 1718 | CD2 | LEU | 1108 | 82.473 | 70.079 | 36.506 | 1.00 | 20.86 |
| ATOM | 1719 | C | LEU | 1108 | 85.781 | 72.524 | 35.686 | 1.00 | 22.72 |
| ATOM | 1720 | O | LEU | 1108 | 86.206 | 73.608 | 35.285 | 1.00 | 24.88 |
| ATOM | 1721 | N | VAL | 1109 | 86.413 | 71.375 | 35.495 | 1.00 | 20.91 |
| ATOM | 1722 | CA | VAL | 1109 | 87.695 | 71.260 | 34.820 | 1.00 | 20.17 |
| ATOM | 1723 | CB | VAL | 1109 | 88.855 | 71.399 | 35.833 | 1.00 | 21.15 |
| ATOM | 1724 | CG1 | VAL | 1109 | 90.117 | 70.788 | 35.292 | 1.00 | 22.22 |
| ATOM | 1725 | CG2 | VAL | 1109 | 89.092 | 72.858 | 36.156 | 1.00 | 22.70 |
| ATOM | 1726 | C | VAL | 1109 | 87.674 | 69.850 | 34.245 | 1.00 | 19.05 |
| ATOM | 1727 | O | VAL | 1109 | 87.065 | 68.967 | 34.839 | 1.00 | 19.81 |
| ATOM | 1728 | N | GLY | 1110 | 88.306 | 69.648 | 33.092 | 1.00 | 17.18 |
| ATOM | 1729 | CA | GLY | 1110 | 88.328 | 68.334 | 32.477 | 1.00 | 16.06 |
| ATOM | 1730 | C | GLY | 1110 | 89.518 | 68.134 | 31.558 | 1.00 | 17.59 |
| ATOM | 1731 | O | GLY | 1110 | 89.896 | 69.050 | 30.823 | 1.00 | 16.16 |
| ATOM | 1732 | N | TRP | 1111 | 90.139 | 66.957 | 31.650 | 1.00 | 17.19 |
| ATOM | 1733 | CA | TRP | 1111 | 91.299 | 66.569 | 30.835 | 1.00 | 16.21 |
| ATOM | 1734 | CB | TRP | 1111 | 92.498 | 66.181 | 31.721 | 1.00 | 14.75 |
| ATOM | 1735 | CG | TRP | 1111 | 93.039 | 67.225 | 32.642 | 1.00 | 11.64 |
| ATOM | 1736 | CD2 | TRP | 1111 | 92.802 | 67.337 | 34.058 | 1.00 | 11.04 |
| ATOM | 1737 | CE2 | TRP | 1111 | 93.577 | 68.419 | 34.525 | 1.00 | 11.37 |
| ATOM | 1738 | CE3 | TRP | 1111 | 92.011 | 66.626 | 34.973 | 1.00 | 13.68 |
| ATOM | 1739 | CD1 | TRP | 1111 | 93.916 | 68.213 | 32.321 | 1.00 | 11.69 |
| ATOM | 1740 | NE1 | TRP | 1111 | 94.247 | 68.935 | 33.447 | 1.00 | 14.19 |
| ATOM | 1741 | CZ2 | TRP | 1111 | 93.589 | 68.809 | 35.867 | 1.00 | 11.96 |
| ATOM | 1742 | CZ3 | TRP | 1111 | 92.022 | 67.011 | 36.308 | 1.00 | 11.51 |
| ATOM | 1743 | CH2 | TRP | 1111 | 92.808 | 68.095 | 36.741 | 1.00 | 13.13 |
| ATOM | 1744 | C | TRP | 1111 | 90.873 | 65.290 | 30.125 | 1.00 | 17.82 |
| ATOM | 1745 | O | TRP | 1111 | 89.882 | 64.670 | 30.516 | 1.00 | 20.28 |
| ATOM | 1746 | N | PRO | 1112 | 91.581 | 64.885 | 29.053 | 1.00 | 18.22 |
| ATOM | 1747 | CD | PRO | 1112 | 92.711 | 65.493 | 28.331 | 1.00 | 17.52 |
| ATOM | 1748 | CA | PRO | 1112 | 91.153 | 63.637 | 28.406 | 1.00 | 16.49 |
| ATOM | 1749 | CB | PRO | 1112 | 92.189 | 63.452 | 27.309 | 1.00 | 15.54 |
| ATOM | 1750 | CG | PRO | 1112 | 92.586 | 64.846 | 26.978 | 1.00 | 18.88 |
| ATOM | 1751 | C | PRO | 1112 | 91.318 | 62.567 | 29.477 | 1.00 | 18.48 |
| ATOM | 1752 | O | PRO | 1112 | 92.207 | 62.679 | 30.322 | 1.00 | 21.84 |
| ATOM | 1753 | N | ALA | 1113 | 90.443 | 61.573 | 29.512 | 1.00 | 19.42 |
| ATOM | 1754 | CA | ALA | 1113 | 90.572 | 60.540 | 30.526 | 1.00 | 18.50 |
| ATOM | 1755 | CB | ALA | 1113 | 89.441 | 59.543 | 30.420 | 1.00 | 17.46 |
| ATOM | 1756 | C | ALA | 1113 | 91.909 | 59.851 | 30.319 | 1.00 | 20.35 |
| ATOM | 1757 | O | ALA | 1113 | 92.278 | 59.532 | 29.189 | 1.00 | 21.19 |
| ATOM | 1758 | N | PRO | 1114 | 92.689 | 59.681 | 31.396 | 1.00 | 21.47 |
| ATOM | 1759 | CD | PRO | 1114 | 92.488 | 60.128 | 32.783 | 1.00 | 22.45 |
| ATOM | 1760 | CA | PRO | 1114 | 93.984 | 59.022 | 31.250 | 1.00 | 22.96 |
| ATOM | 1761 | CB | PRO | 1114 | 94.529 | 59.018 | 32.682 | 1.00 | 23.65 |

FIGURE 3 (CONT.)

| ATOM | 1762 | CG | PRO | 1114 | 93.306 | 59.138 | 33.537 | 1.00 | 22.54 |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 1763 | C | PRO | 1114 | 93.835 | 57.620 | 30.693 | 1.00 | 24.51 |
| ATOM | 1764 | O | PRO | 1114 | 92.888 | 56.903 | 31.024 | 1.00 | 26.99 |
| ATOM | 1765 | N | GLN | 1115 | 94.730 | 57.254 | 29.786 | 1.00 | 26.09 |
| ATOM | 1766 | CA | GLN | 1115 | 94.706 | 55.925 | 29.195 | 1.00 | 28.46 |
| ATOM | 1767 | CB | GLN | 1115 | 95.903 | 55.744 | 28.258 | 1.00 | 30.59 |
| ATOM | 1768 | CG | GLN | 1115 | 95.895 | 56.656 | 27.033 | 1.00 | 34.32 |
| ATOM | 1769 | CD | GLN | 1115 | 94.865 | 56.236 | 26.009 | 1.00 | 37.60 |
| ATOM | 1770 | OE1 | GLN | 1115 | 94.731 | 55.051 | 25.699 | 1.00 | 39.96 |
| ATOM | 1771 | NE2 | GLN | 1115 | 94.122 | 57.203 | 25.479 | 1.00 | 41.37 |
| ATOM | 1772 | C | GLN | 1115 | 94.762 | 54.895 | 30.325 | 1.00 | 28.93 |
| ATOM | 1773 | O | GLN | 1115 | 95.548 | 55.039 | 31.269 | 1.00 | 29.99 |
| ATOM | 1774 | N | GLY | 1116 | 93.881 | 53.902 | 30.257 | 1.00 | 28.45 |
| ATOM | 1775 | CA | GLY | 1116 | 93.842 | 52.862 | 31.272 | 1.00 | 28.19 |
| ATOM | 1776 | C | GLY | 1116 | 92.595 | 52.883 | 32.140 | 1.00 | 28.90 |
| ATOM | 1777 | O | GLY | 1116 | 92.155 | 51.840 | 32.633 | 1.00 | 30.64 |
| ATOM | 1778 | N | SER | 1117 | 92.027 | 54.071 | 32.327 | 1.00 | 28.03 |
| ATOM | 1779 | CA | SER | 1117 | 90.834 | 54.246 | 33.143 | 1.00 | 25.22 |
| ATOM | 1780 | CB | SER | 1117 | 90.688 | 55.717 | 33.517 | 1.00 | 21.89 |
| ATOM | 1781 | OG | SER | 1117 | 90.524 | 56.491 | 32.349 | 1.00 | 17.60 |
| ATOM | 1782 | C | SER | 1117 | 89.567 | 53.784 | 32.432 | 1.00 | 25.37 |
| ATOM | 1783 | O | SER | 1117 | 89.592 | 53.456 | 31.241 | 1.00 | 26.03 |
| ATOM | 1784 | N | ARG | 1118 | 88.468 | 53.734 | 33.181 | 1.00 | 25.35 |
| ATOM | 1785 | CA | ARG | 1118 | 87.170 | 53.350 | 32.641 | 1.00 | 25.91 |
| ATOM | 1786 | CB | ARG | 1118 | 86.635 | 52.074 | 33.300 | 1.00 | 31.51 |
| ATOM | 1787 | CG | ARG | 1118 | 87.368 | 50.796 | 32.919 | 1.00 | 42.46 |
| ATOM | 1788 | CD | ARG | 1118 | 87.604 | 50.721 | 31.414 | 1.00 | 51.80 |
| ATOM | 1789 | NE | ARG | 1118 | 87.874 | 49.357 | 30.956 | 1.00 | 61.09 |
| ATOM | 1790 | CZ | ARG | 1118 | 88.830 | 49.022 | 30.090 | 1.00 | 65.33 |
| ATOM | 1791 | NH1 | ARG | 1118 | 88.981 | 47.749 | 29.738 | 1.00 | 68.07 |
| ATOM | 1792 | NH2 | ARG | 1118 | 89.661 | 49.941 | 29.606 | 1.00 | 67.27 |
| ATOM | 1793 | C | ARG | 1118 | 86.252 | 54.515 | 32.960 | 1.00 | 24.68 |
| ATOM | 1794 | O | ARG | 1118 | 86.375 | 55.128 | 34.020 | 1.00 | 24.68 |
| ATOM | 1795 | N | SER | 1119 | 85.355 | 54.844 | 32.043 | 1.00 | 22.26 |
| ATOM | 1796 | CA | SER | 1119 | 84.446 | 55.957 | 32.263 | 1.00 | 22.87 |
| ATOM | 1797 | CB | SER | 1119 | 84.333 | 56.807 | 30.993 | 1.00 | 21.77 |
| ATOM | 1798 | OG | SER | 1119 | 85.535 | 57.511 | 30.735 | 1.00 | 26.02 |
| ATOM | 1799 | C | SER | 1119 | 83.053 | 55.536 | 32.692 | 1.00 | 20.90 |
| ATOM | 1800 | O | SER | 1119 | 82.620 | 54.421 | 32.425 | 1.00 | 21.97 |
| ATOM | 1801 | N | LEU | 1120 | 82.379 | 56.424 | 33.409 | 1.00 | 19.67 |
| ATOM | 1802 | CA | LEU | 1120 | 81.008 | 56.195 | 33.827 | 1.00 | 16.91 |
| ATOM | 1803 | CB | LEU | 1120 | 80.691 | 56.939 | 35.131 | 1.00 | 13.88 |
| ATOM | 1804 | CG | LEU | 1120 | 81.329 | 56.564 | 36.469 | 1.00 | 11.68 |
| ATOM | 1805 | CD1 | LEU | 1120 | 80.978 | 57.623 | 37.470 | 1.00 | 11.76 |
| ATOM | 1806 | CD2 | LEU | 1120 | 80.854 | 55.209 | 36.950 | 1.00 | 13.04 |
| ATOM | 1807 | C | LEU | 1120 | 80.197 | 56.828 | 32.704 | 1.00 | 16.42 |
| ATOM | 1808 | O | LEU | 1120 | 80.753 | 57.509 | 31.840 | 1.00 | 15.05 |
| ATOM | 1809 | N | THR | 1121 | 78.893 | 56.602 | 32.714 | 1.00 | 18.09 |
| ATOM | 1810 | CA | THR | 1121 | 78.012 | 57.189 | 31.719 | 1.00 | 19.50 |
| ATOM | 1811 | CB | THR | 1121 | 77.383 | 56.120 | 30.825 | 1.00 | 20.88 |
| ATOM | 1812 | OG1 | THR | 1121 | 77.011 | 54.987 | 31.620 | 1.00 | 26.65 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1813 | CG2 | THR | 1121 | 78.372 | 55.683 | 29.758 | 1.00 | 21.77 |
| ATOM | 1814 | C | THR | 1121 | 76.938 | 57.941 | 32.485 | 1.00 | 18.52 |
| ATOM | 1815 | O | THR | 1121 | 76.613 | 57.579 | 33.616 | 1.00 | 20.72 |
| ATOM | 1816 | N | PRO | 1122 | 76.441 | 59.052 | 31.931 | 1.00 | 18.23 |
| ATOM | 1817 | CD | PRO | 1122 | 76.865 | 59.703 | 30.680 | 1.00 | 17.02 |
| ATOM | 1818 | CA | PRO | 1122 | 75.403 | 59.835 | 32.606 | 1.00 | 18.29 |
| ATOM | 1819 | CB | PRO | 1122 | 75.108 | 60.939 | 31.600 | 1.00 | 18.11 |
| ATOM | 1820 | CG | PRO | 1122 | 76.432 | 61.122 | 30.908 | 1.00 | 16.83 |
| ATOM | 1821 | C | PRO | 1122 | 74.153 | 59.019 | 32.931 | 1.00 | 20.74 |
| ATOM | 1822 | O | PRO | 1122 | 73.887 | 57.985 | 32.317 | 1.00 | 22.14 |
| ATOM | 1823 | N | CYS | 1123 | 73.405 | 59.476 | 33.925 | 1.00 | 23.09 |
| ATOM | 1824 | CA | CYS | 1123 | 72.184 | 58.807 | 34.348 | 1.00 | 25.58 |
| ATOM | 1825 | CB | CYS | 1123 | 71.811 | 59.265 | 35.759 | 1.00 | 25.03 |
| ATOM | 1826 | SG | CYS | 1123 | 70.363 | 58.469 | 36.474 | 1.00 | 22.23 |
| ATOM | 1827 | C | CYS | 1123 | 71.069 | 59.169 | 33.381 | 1.00 | 27.87 |
| ATOM | 1828 | O | CYS | 1123 | 70.978 | 60.314 | 32.942 | 1.00 | 29.71 |
| ATOM | 1829 | N | THR | 1124 | 70.211 | 58.199 | 33.075 | 1.00 | 30.25 |
| ATOM | 1830 | CA | THR | 1124 | 69.086 | 58.398 | 32.162 | 1.00 | 30.66 |
| ATOM | 1831 | CB | THR | 1124 | 69.407 | 57.845 | 30.756 | 1.00 | 29.19 |
| ATOM | 1832 | OG1 | THR | 1124 | 69.987 | 56.537 | 30.874 | 1.00 | 28.07 |
| ATOM | 1833 | CG2 | THR | 1124 | 70.354 | 58.776 | 30.009 | 1.00 | 26.85 |
| ATOM | 1834 | C | THR | 1124 | 67.853 | 57.684 | 32.720 | 1.00 | 32.73 |
| ATOM | 1835 | O | THR | 1124 | 67.224 | 56.867 | 32.049 | 1.00 | 35.79 |
| ATOM | 1836 | N | CYS | 1125 | 67.532 | 57.980 | 33.971 | 1.00 | 33.01 |
| ATOM | 1837 | CA | CYS | 1125 | 66.395 | 57.373 | 34.639 | 1.00 | 32.02 |
| ATOM | 1838 | CB | CYS | 1125 | 66.836 | 56.136 | 35.433 | 1.00 | 33.60 |
| ATOM | 1839 | SG | CYS | 1125 | 67.885 | 56.458 | 36.910 | 1.00 | 37.33 |
| ATOM | 1840 | C | CYS | 1125 | 65.785 | 58.403 | 35.571 | 1.00 | 31.70 |
| ATOM | 1841 | O | CYS | 1125 | 64.771 | 58.151 | 36.211 | 1.00 | 35.06 |
| ATOM | 1842 | N | GLY | 1126 | 66.417 | 59.569 | 35.642 | 1.00 | 30.53 |
| ATOM | 1843 | CA | GLY | 1126 | 65.927 | 60.636 | 36.490 | 1.00 | 30.87 |
| ATOM | 1844 | C | GLY | 1126 | 65.769 | 60.278 | 37.954 | 1.00 | 30.72 |
| ATOM | 1845 | O | GLY | 1126 | 65.092 | 60.991 | 38.691 | 1.00 | 33.42 |
| ATOM | 1846 | N | SER | 1127 | 66.408 | 59.200 | 38.394 | 1.00 | 29.86 |
| ATOM | 1847 | CA | SER | 1127 | 66.297 | 58.790 | 39.786 | 1.00 | 29.79 |
| ATOM | 1848 | CB | SER | 1127 | 67.098 | 57.519 | 40.045 | 1.00 | 28.49 |
| ATOM | 1849 | OG | SER | 1127 | 67.027 | 57.174 | 41.421 | 1.00 | 30.28 |
| ATOM | 1850 | C | SER | 1127 | 66.718 | 59.881 | 40.771 | 1.00 | 31.88 |
| ATOM | 1851 | O | SER | 1127 | 67.629 | 60.673 | 40.499 | 1.00 | 31.79 |
| ATOM | 1852 | N | SER | 1128 | 66.045 | 59.908 | 41.917 | 1.00 | 32.25 |
| ATOM | 1853 | CA | SER | 1128 | 66.335 | 60.884 | 42.957 | 1.00 | 32.78 |
| ATOM | 1854 | CB | SER | 1128 | 65.045 | 61.545 | 43.431 | 1.00 | 34.11 |
| ATOM | 1855 | OG | SER | 1128 | 64.117 | 60.564 | 43.869 | 1.00 | 38.32 |
| ATOM | 1856 | C | SER | 1128 | 67.061 | 60.246 | 44.139 | 1.00 | 31.47 |
| ATOM | 1857 | O | SER | 1128 | 67.345 | 60.924 | 45.130 | 1.00 | 30.85 |
| ATOM | 1858 | N | ASP | 1129 | 67.293 | 58.936 | 44.066 | 1.00 | 29.87 |
| ATOM | 1859 | CA | ASP | 1129 | 68.012 | 58.219 | 45.123 | 1.00 | 29.89 |
| ATOM | 1860 | CB | ASP | 1129 | 67.408 | 56.839 | 45.348 | 1.00 | 31.52 |
| ATOM | 1861 | CG | ASP | 1129 | 65.931 | 56.898 | 45.658 | 1.00 | 34.71 |
| ATOM | 1862 | OD1 | ASP | 1129 | 65.561 | 57.534 | 46.667 | 1.00 | 36.72 |
| ATOM | 1863 | OD2 | ASP | 1129 | 65.141 | 56.320 | 44.878 | 1.00 | 35.48 |

42/60

FIGURE 3 (CONT.)

| ATOM | 1864 | C | ASP | 1129 | 69.442 | 58.075 | 44.624 | 1.00 | 29.13 |
|------|------|---|-----|------|--------|--------|--------|------|-------|
| ATOM | 1865 | O | ASP | 1129 | 69.711 | 57.254 | 43.745 | 1.00 | 28.49 |
| ATOM | 1866 | N | LEU | 1130 | 70.342 | 58.886 | 45.177 | 1.00 | 27.18 |
| ATOM | 1867 | CA | LEU | 1130 | 71.740 | 58.907 | 44.760 | 1.00 | 24.28 |
| ATOM | 1868 | CB | LEU | 1130 | 72.156 | 60.349 | 44.445 | 1.00 | 23.07 |
| ATOM | 1869 | CG | LEU | 1130 | 71.172 | 61.255 | 43.689 | 1.00 | 21.59 |
| ATOM | 1870 | CD1 | LEU | 1130 | 71.727 | 62.664 | 43.589 | 1.00 | 19.14 |
| ATOM | 1871 | CD2 | LEU | 1130 | 70.883 | 60.693 | 42.319 | 1.00 | 19.32 |
| ATOM | 1872 | C | LEU | 1130 | 72.690 | 58.324 | 45.802 | 1.00 | 23.34 |
| ATOM | 1873 | O | LEU | 1130 | 72.347 | 58.198 | 46.979 | 1.00 | 24.14 |
| ATOM | 1874 | N | TYR | 1131 | 73.898 | 57.988 | 45.360 | 1.00 | 23.40 |
| ATOM | 1875 | CA | TYR | 1131 | 74.928 | 57.423 | 46.225 | 1.00 | 22.86 |
| ATOM | 1876 | CB | TYR | 1131 | 75.039 | 55.924 | 45.980 | 1.00 | 22.51 |
| ATOM | 1877 | CG | TYR | 1131 | 73.719 | 55.224 | 46.135 | 1.00 | 21.96 |
| ATOM | 1878 | CD1 | TYR | 1131 | 72.923 | 54.955 | 45.034 | 1.00 | 21.81 |
| ATOM | 1879 | CE1 | TYR | 1131 | 71.671 | 54.382 | 45.176 | 1.00 | 22.83 |
| ATOM | 1880 | CD2 | TYR | 1131 | 73.234 | 54.893 | 47.393 | 1.00 | 24.12 |
| ATOM | 1881 | CE2 | TYR | 1131 | 71.985 | 54.318 | 47.551 | 1.00 | 24.94 |
| ATOM | 1882 | CZ | TYR | 1131 | 71.205 | 54.065 | 46.437 | 1.00 | 24.69 |
| ATOM | 1883 | OH | TYR | 1131 | 69.951 | 53.504 | 46.590 | 1.00 | 26.44 |
| ATOM | 1884 | C | TYR | 1131 | 76.268 | 58.108 | 45.965 | 1.00 | 22.03 |
| ATOM | 1885 | O | TYR | 1131 | 76.773 | 58.088 | 44.847 | 1.00 | 22.92 |
| ATOM | 1886 | N | LEU | 1132 | 76.809 | 58.737 | 47.003 | 1.00 | 21.21 |
| ATOM | 1887 | CA | LEU | 1132 | 78.071 | 59.463 | 46.956 | 1.00 | 20.60 |
| ATOM | 1888 | CB | LEU | 1132 | 78.032 | 60.576 | 48.007 | 1.00 | 21.28 |
| ATOM | 1889 | CG | LEU | 1132 | 78.843 | 61.874 | 47.906 | 1.00 | 23.35 |
| ATOM | 1890 | CD1 | LEU | 1132 | 78.614 | 62.661 | 49.172 | 1.00 | 25.61 |
| ATOM | 1891 | CD2 | LEU | 1132 | 80.319 | 61.623 | 47.741 | 1.00 | 26.41 |
| ATOM | 1892 | C | LEU | 1132 | 79.249 | 58.541 | 47.263 | 1.00 | 20.51 |
| ATOM | 1893 | O | LEU | 1132 | 79.250 | 57.853 | 48.283 | 1.00 | 23.83 |
| ATOM | 1894 | N | VAL | 1133 | 80.246 | 58.524 | 46.386 | 1.00 | 18.28 |
| ATOM | 1895 | CA | VAL | 1133 | 81.438 | 57.714 | 46.592 | 1.00 | 16.12 |
| ATOM | 1896 | CB | VAL | 1133 | 81.912 | 57.067 | 45.284 | 1.00 | 14.27 |
| ATOM | 1897 | CG1 | VAL | 1133 | 83.198 | 56.291 | 45.516 | 1.00 | 11.21 |
| ATOM | 1898 | CG2 | VAL | 1133 | 80.821 | 56.165 | 44.722 | 1.00 | 9.93 |
| ATOM | 1899 | C | VAL | 1133 | 82.538 | 58.635 | 47.130 | 1.00 | 20.05 |
| ATOM | 1900 | O | VAL | 1133 | 83.051 | 59.504 | 46.411 | 1.00 | 18.89 |
| ATOM | 1901 | N | THR | 1134 | 82.861 | 58.471 | 48.410 | 1.00 | 21.68 |
| ATOM | 1902 | CA | THR | 1134 | 83.876 | 59.286 | 49.061 | 1.00 | 21.80 |
| ATOM | 1903 | CB | THR | 1134 | 83.741 | 59.227 | 50.584 | 1.00 | 19.89 |
| ATOM | 1904 | OG1 | THR | 1134 | 84.183 | 57.946 | 51.043 | 1.00 | 21.40 |
| ATOM | 1905 | CG2 | THR | 1134 | 82.292 | 59.428 | 50.999 | 1.00 | 18.10 |
| ATOM | 1906 | C | THR | 1134 | 85.296 | 58.872 | 48.705 | 1.00 | 24.10 |
| ATOM | 1907 | O | THR | 1134 | 85.530 | 57.792 | 48.166 | 1.00 | 24.71 |
| ATOM | 1908 | N | ARG | 1135 | 86.245 | 59.719 | 49.083 | 1.00 | 26.05 |
| ATOM | 1909 | CA | ARG | 1135 | 87.665 | 59.488 | 48.840 | 1.00 | 28.72 |
| ATOM | 1910 | CB | ARG | 1135 | 88.472 | 60.667 | 49.386 | 1.00 | 32.63 |
| ATOM | 1911 | CG | ARG | 1135 | 89.950 | 60.546 | 49.160 | 1.00 | 35.08 |
| ATOM | 1912 | CD | ARG | 1135 | 90.705 | 61.556 | 49.968 | 1.00 | 39.19 |
| ATOM | 1913 | NE | ARG | 1135 | 92.134 | 61.292 | 49.896 | 1.00 | 46.35 |
| ATOM | 1914 | CZ | ARG | 1135 | 93.018 | 61.704 | 50.798 | 1.00 | 53.28 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1915 | NH1 | ARG | 1135 | 94.305 | 61.414 | 50.643 | 1.00 | 56.95 |
| ATOM | 1916 | NH2 | ARG | 1135 | 92.618 | 62.396 | 51.862 | 1.00 | 57.23 |
| ATOM | 1917 | C | ARG | 1135 | 88.173 | 58.202 | 49.487 | 1.00 | 27.12 |
| ATOM | 1918 | O | ARG | 1135 | 89.205 | 57.668 | 49.094 | 1.00 | 28.70 |
| ATOM | 1919 | N | HIS | 1136 | 87.471 | 57.732 | 50.508 | 1.00 | 26.02 |
| ATOM | 1920 | CA | HIS | 1136 | 87.875 | 56.517 | 51.201 | 1.00 | 25.17 |
| ATOM | 1921 | CB | HIS | 1136 | 87.613 | 56.649 | 52.695 | 1.00 | 27.11 |
| ATOM | 1922 | CG | HIS | 1136 | 88.126 | 57.929 | 53.272 | 1.00 | 33.56 |
| ATOM | 1923 | CD2 | HIS | 1136 | 87.473 | 59.032 | 53.704 | 1.00 | 37.55 |
| ATOM | 1924 | ND1 | HIS | 1136 | 89.473 | 58.206 | 53.392 | 1.00 | 35.53 |
| ATOM | 1925 | CE1 | HIS | 1136 | 89.626 | 59.429 | 53.869 | 1.00 | 38.38 |
| ATOM | 1926 | NE2 | HIS | 1136 | 88.429 | 59.954 | 54.068 | 1.00 | 39.18 |
| ATOM | 1927 | C | HIS | 1136 | 87.150 | 55.306 | 50.645 | 1.00 | 24.36 |
| ATOM | 1928 | O | HIS | 1136 | 87.172 | 54.236 | 51.252 | 1.00 | 24.55 |
| ATOM | 1929 | N | ALA | 1137 | 86.522 | 55.480 | 49.485 | 1.00 | 21.92 |
| ATOM | 1930 | CA | ALA | 1137 | 85.796 | 54.413 | 48.823 | 1.00 | 20.47 |
| ATOM | 1931 | CB | ALA | 1137 | 86.728 | 53.257 | 48.511 | 1.00 | 20.48 |
| ATOM | 1932 | C | ALA | 1137 | 84.588 | 53.934 | 49.623 | 1.00 | 21.30 |
| ATOM | 1933 | O | ALA | 1137 | 84.316 | 52.734 | 49.719 | 1.00 | 22.24 |
| ATOM | 1934 | N | ASP | 1138 | 83.876 | 54.880 | 50.218 | 1.00 | 21.09 |
| ATOM | 1935 | CA | ASP | 1138 | 82.674 | 54.569 | 50.973 | 1.00 | 21.30 |
| ATOM | 1936 | CB | ASP | 1138 | 82.662 | 55.283 | 52.325 | 1.00 | 20.40 |
| ATOM | 1937 | CG | ASP | 1138 | 83.685 | 54.731 | 53.291 | 1.00 | 20.82 |
| ATOM | 1938 | OD1 | ASP | 1138 | 83.890 | 53.501 | 53.319 | 1.00 | 23.51 |
| ATOM | 1939 | OD2 | ASP | 1138 | 84.287 | 55.527 | 54.034 | 1.00 | 23.93 |
| ATOM | 1940 | C | ASP | 1138 | 81.537 | 55.097 | 50.119 | 1.00 | 23.33 |
| ATOM | 1941 | O | ASP | 1138 | 81.646 | 56.183 | 49.546 | 1.00 | 25.82 |
| ATOM | 1942 | N | VAL | 1139 | 80.468 | 54.320 | 50.003 | 1.00 | 23.72 |
| ATOM | 1943 | CA | VAL | 1139 | 79.305 | 54.702 | 49.214 | 1.00 | 20.95 |
| ATOM | 1944 | CB | VAL | 1139 | 78.779 | 53.501 | 48.415 | 1.00 | 18.28 |
| ATOM | 1945 | CG1 | VAL | 1139 | 77.527 | 53.875 | 47.661 | 1.00 | 15.80 |
| ATOM | 1946 | CG2 | VAL | 1139 | 79.857 | 52.982 | 47.481 | 1.00 | 12.00 |
| ATOM | 1947 | C | VAL | 1139 | 78.251 | 55.125 | 50.208 | 1.00 | 22.42 |
| ATOM | 1948 | O | VAL | 1139 | 77.814 | 54.316 | 51.017 | 1.00 | 25.81 |
| ATOM | 1949 | N | ILE | 1140 | 77.862 | 56.389 | 50.188 | 1.00 | 23.66 |
| ATOM | 1950 | CA | ILE | 1140 | 76.854 | 56.863 | 51.130 | 1.00 | 25.17 |
| ATOM | 1951 | CB | ILE | 1140 | 77.449 | 57.935 | 52.089 | 1.00 | 26.79 |
| ATOM | 1952 | CG2 | ILE | 1140 | 78.669 | 57.368 | 52.805 | 1.00 | 27.35 |
| ATOM | 1953 | CG1 | ILE | 1140 | 77.887 | 59.188 | 51.330 | 1.00 | 28.07 |
| ATOM | 1954 | CD1 | ILE | 1140 | 78.560 | 60.238 | 52.219 | 1.00 | 27.71 |
| ATOM | 1955 | C | ILE | 1140 | 75.607 | 57.375 | 50.408 | 1.00 | 25.17 |
| ATOM | 1956 | O | ILE | 1140 | 75.717 | 58.102 | 49.433 | 1.00 | 25.94 |
| ATOM | 1957 | N | PRO | 1141 | 74.406 | 56.943 | 50.834 | 1.00 | 25.23 |
| ATOM | 1958 | CD | PRO | 1141 | 74.102 | 56.065 | 51.974 | 1.00 | 26.31 |
| ATOM | 1959 | CA | PRO | 1141 | 73.167 | 57.388 | 50.189 | 1.00 | 26.02 |
| ATOM | 1960 | CB | PRO | 1141 | 72.099 | 56.552 | 50.887 | 1.00 | 26.05 |
| ATOM | 1961 | CG | PRO | 1141 | 72.647 | 56.404 | 52.253 | 1.00 | 26.71 |
| ATOM | 1962 | C | PRO | 1141 | 72.912 | 58.874 | 50.384 | 1.00 | 27.84 |
| ATOM | 1963 | O | PRO | 1141 | 73.231 | 59.440 | 51.432 | 1.00 | 29.15 |
| ATOM | 1964 | N | VAL | 1142 | 72.289 | 59.483 | 49.383 | 1.00 | 28.51 |
| ATOM | 1965 | CA | VAL | 1142 | 71.973 | 60.902 | 49.385 | 1.00 | 27.59 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1966 | CB | VAL | 1142 | 73.080 | 61.695 | 48.640 | 1.00 | 26.82 |
| ATOM | 1967 | CG1 | VAL | 1142 | 72.710 | 63.160 | 48.504 | 1.00 | 25.54 |
| ATOM | 1968 | CG2 | VAL | 1142 | 74.398 | 61.554 | 49.368 | 1.00 | 24.22 |
| ATOM | 1969 | C | VAL | 1142 | 70.650 | 61.047 | 48.640 | 1.00 | 30.42 |
| ATOM | 1970 | O | VAL | 1142 | 70.465 | 60.445 | 47.575 | 1.00 | 31.72 |
| ATOM | 1971 | N | ARG | 1143 | 69.708 | 61.788 | 49.220 | 1.00 | 32.81 |
| ATOM | 1972 | CA | ARG | 1143 | 68.411 | 62.006 | 48.580 | 1.00 | 33.55 |
| ATOM | 1973 | CB | ARG | 1143 | 67.282 | 62.037 | 49.613 | 1.00 | 35.71 |
| ATOM | 1974 | CG | ARG | 1143 | 65.903 | 62.331 | 49.017 | 1.00 | 37.69 |
| ATOM | 1975 | CD | ARG | 1143 | 65.465 | 61.288 | 47.991 | 1.00 | 39.30 |
| ATOM | 1976 | NE | ARG | 1143 | 64.225 | 61.685 | 47.311 | 1.00 | 43.20 |
| ATOM | 1977 | CZ | ARG | 1143 | 63.383 | 60.843 | 46.711 | 1.00 | 43.40 |
| ATOM | 1978 | NH1 | ARG | 1143 | 63.628 | 59.539 | 46.696 | 1.00 | 43.88 |
| ATOM | 1979 | NH2 | ARG | 1143 | 62.297 | 61.307 | 46.108 | 1.00 | 43.09 |
| ATOM | 1980 | C | ARG | 1143 | 68.439 | 63.320 | 47.818 | 1.00 | 33.27 |
| ATOM | 1981 | O | ARG | 1143 | 68.794 | 64.353 | 48.382 | 1.00 | 33.50 |
| ATOM | 1982 | N | ARG | 1144 | 68.044 | 63.280 | 46.549 | 1.00 | 33.18 |
| ATOM | 1983 | CA | ARG | 1144 | 68.038 | 64.471 | 45.709 | 1.00 | 34.20 |
| ATOM | 1984 | CB | ARG | 1144 | 67.725 | 64.089 | 44.260 | 1.00 | 32.94 |
| ATOM | 1985 | CG | ARG | 1144 | 68.475 | 64.900 | 43.203 | 1.00 | 32.47 |
| ATOM | 1986 | CD | ARG | 1144 | 67.952 | 64.546 | 41.815 | 1.00 | 32.92 |
| ATOM | 1987 | NE | ARG | 1144 | 68.924 | 64.732 | 40.738 | 1.00 | 33.75 |
| ATOM | 1988 | CZ | ARG | 1144 | 69.459 | 65.898 | 40.387 | 1.00 | 35.07 |
| ATOM | 1989 | NH1 | ARG | 1144 | 69.125 | 67.007 | 41.029 | 1.00 | 36.60 |
| ATOM | 1990 | NH2 | ARG | 1144 | 70.321 | 65.959 | 39.378 | 1.00 | 35.64 |
| ATOM | 1991 | C | ARG | 1144 | 67.001 | 65.467 | 46.227 | 1.00 | 35.48 |
| ATOM | 1992 | O | ARG | 1144 | 65.825 | 65.139 | 46.374 | 1.00 | 36.95 |
| ATOM | 1993 | N | ARG | 1145 | 67.449 | 66.670 | 46.546 | 1.00 | 36.40 |
| ATOM | 1994 | CA | ARG | 1145 | 66.552 | 67.700 | 47.048 | 1.00 | 37.95 |
| ATOM | 1995 | CB | ARG | 1145 | 67.025 | 68.213 | 48.414 | 1.00 | 37.18 |
| ATOM | 1996 | CG | ARG | 1145 | 66.975 | 67.184 | 49.514 | 1.00 | 36.94 |
| ATOM | 1997 | CD | ARG | 1145 | 65.570 | 66.667 | 49.681 | 1.00 | 38.43 |
| ATOM | 1998 | NE | ARG | 1145 | 65.447 | 65.729 | 50.791 | 1.00 | 41.86 |
| ATOM | 1999 | CZ | ARG | 1145 | 64.341 | 65.043 | 51.062 | 1.00 | 43.83 |
| ATOM | 2000 | NH1 | ARG | 1145 | 63.263 | 65.187 | 50.299 | 1.00 | 46.04 |
| ATOM | 2001 | NH2 | ARG | 1145 | 64.306 | 64.223 | 52.102 | 1.00 | 45.68 |
| ATOM | 2002 | C | ARG | 1145 | 66.507 | 68.856 | 46.063 | 1.00 | 39.67 |
| ATOM | 2003 | O | ARG | 1145 | 66.247 | 70.000 | 46.449 | 1.00 | 42.26 |
| ATOM | 2004 | N | GLY | 1146 | 66.789 | 68.565 | 44.797 | 1.00 | 39.96 |
| ATOM | 2005 | CA | GLY | 1146 | 66.779 | 69.605 | 43.788 | 1.00 | 40.13 |
| ATOM | 2006 | C | GLY | 1146 | 67.932 | 69.428 | 42.823 | 1.00 | 40.68 |
| ATOM | 2007 | O | GLY | 1146 | 68.829 | 68.621 | 43.061 | 1.00 | 41.79 |
| ATOM | 2008 | N | ALA | 1147 | 67.937 | 70.228 | 41.765 | 1.00 | 40.55 |
| ATOM | 2009 | CA | ALA | 1147 | 68.961 | 70.157 | 40.733 | 1.00 | 39.49 |
| ATOM | 2010 | CB | ALA | 1147 | 68.890 | 71.392 | 39.834 | 1.00 | 40.92 |
| ATOM | 2011 | C | ALA | 1147 | 70.392 | 69.927 | 41.214 | 1.00 | 38.50 |
| ATOM | 2012 | O | ALA | 1147 | 71.068 | 69.024 | 40.717 | 1.00 | 38.36 |
| ATOM | 2013 | N | SER | 1148 | 70.854 | 70.721 | 42.176 | 1.00 | 37.84 |
| ATOM | 2014 | CA | SER | 1148 | 72.222 | 70.564 | 42.656 | 1.00 | 36.96 |
| ATOM | 2015 | CB | SER | 1148 | 73.097 | 71.732 | 42.182 | 1.00 | 36.77 |
| ATOM | 2016 | OG | SER | 1148 | 72.690 | 72.965 | 42.755 | 1.00 | 40.56 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2017 | C | SER | 1148 | 72.391 | 70.363 | 44.156 | 1.00 | 36.04 |
| ATOM | 2018 | O | SER | 1148 | 73.382 | 70.812 | 44.734 | 1.00 | 36.47 |
| ATOM | 2019 | N | ARG | 1149 | 71.452 | 69.672 | 44.788 | 1.00 | 34.56 |
| ATOM | 2020 | CA | ARG | 1149 | 71.575 | 69.416 | 46.214 | 1.00 | 33.98 |
| ATOM | 2021 | CB | ARG | 1149 | 70.923 | 70.518 | 47.050 | 1.00 | 35.91 |
| ATOM | 2022 | CG | ARG | 1149 | 71.621 | 70.740 | 48.397 | 1.00 | 40.83 |
| ATOM | 2023 | CD | ARG | 1149 | 70.760 | 71.514 | 49.389 | 1.00 | 44.70 |
| ATOM | 2024 | NE | ARG | 1149 | 71.544 | 72.142 | 50.456 | 1.00 | 48.33 |
| ATOM | 2025 | CZ | ARG | 1149 | 71.832 | 73.444 | 50.506 | 1.00 | 50.37 |
| ATOM | 2026 | NH1 | ARG | 1149 | 71.416 | 74.266 | 49.552 | 1.00 | 52.98 |
| ATOM | 2027 | NH2 | ARG | 1149 | 72.508 | 73.941 | 51.531 | 1.00 | 51.44 |
| ATOM | 2028 | C | ARG | 1149 | 70.981 | 68.070 | 46.573 | 1.00 | 32.53 |
| ATOM | 2029 | O | ARG | 1149 | 70.168 | 67.513 | 45.833 | 1.00 | 32.88 |
| ATOM | 2030 | N | GLY | 1150 | 71.418 | 67.541 | 47.705 | 1.00 | 31.86 |
| ATOM | 2031 | CA | GLY | 1150 | 70.934 | 66.260 | 48.171 | 1.00 | 29.91 |
| ATOM | 2032 | C | GLY | 1150 | 71.207 | 66.138 | 49.653 | 1.00 | 28.10 |
| ATOM | 2033 | O | GLY | 1150 | 72.237 | 66.603 | 50.137 | 1.00 | 29.55 |
| ATOM | 2034 | N | SER | 1151 | 70.289 | 65.516 | 50.376 | 1.00 | 27.99 |
| ATOM | 2035 | CA | SER | 1151 | 70.439 | 65.348 | 51.811 | 1.00 | 28.25 |
| ATOM | 2036 | CB | SER | 1151 | 69.072 | 65.434 | 52.487 | 1.00 | 31.79 |
| ATOM | 2037 | OG | SER | 1151 | 68.433 | 66.664 | 52.201 | 1.00 | 39.70 |
| ATOM | 2038 | C | SER | 1151 | 71.071 | 64.020 | 52.164 | 1.00 | 26.53 |
| ATOM | 2039 | O | SER | 1151 | 70.653 | 62.974 | 51.662 | 1.00 | 25.17 |
| ATOM | 2040 | N | LEU | 1152 | 72.089 | 64.055 | 53.013 | 1.00 | 25.87 |
| ATOM | 2041 | CA | LEU | 1152 | 72.706 | 62.814 | 53.443 | 1.00 | 27.78 |
| ATOM | 2042 | CB | LEU | 1152 | 73.948 | 63.075 | 54.296 | 1.00 | 26.21 |
| ATOM | 2043 | CG | LEU | 1152 | 75.157 | 63.729 | 53.627 | 1.00 | 24.51 |
| ATOM | 2044 | CD1 | LEU | 1152 | 76.335 | 63.659 | 54.564 | 1.00 | 23.77 |
| ATOM | 2045 | CD2 | LEU | 1152 | 75.496 | 63.008 | 52.343 | 1.00 | 25.98 |
| ATOM | 2046 | C | LEU | 1152 | 71.629 | 62.147 | 54.287 | 1.00 | 29.68 |
| ATOM | 2047 | O | LEU | 1152 | 70.965 | 62.819 | 55.075 | 1.00 | 31.97 |
| ATOM | 2048 | N | LEU | 1153 | 71.385 | 60.860 | 54.065 | 1.00 | 31.23 |
| ATOM | 2049 | CA | LEU | 1153 | 70.372 | 60.159 | 54.845 | 1.00 | 31.26 |
| ATOM | 2050 | CB | LEU | 1153 | 69.991 | 58.836 | 54.181 | 1.00 | 29.73 |
| ATOM | 2051 | CG | LEU | 1153 | 68.811 | 58.932 | 53.215 | 1.00 | 27.81 |
| ATOM | 2052 | CD1 | LEU | 1153 | 69.023 | 60.036 | 52.193 | 1.00 | 29.89 |
| ATOM | 2053 | CD2 | LEU | 1153 | 68.619 | 57.614 | 52.528 | 1.00 | 28.98 |
| ATOM | 2054 | C | LEU | 1153 | 70.862 | 59.933 | 56.269 | 1.00 | 33.19 |
| ATOM | 2055 | O | LEU | 1153 | 70.075 | 59.670 | 57.182 | 1.00 | 34.12 |
| ATOM | 2056 | N | SER | 1154 | 72.166 | 60.072 | 56.459 | 1.00 | 34.74 |
| ATOM | 2057 | CA | SER | 1154 | 72.775 | 59.899 | 57.762 | 1.00 | 37.99 |
| ATOM | 2058 | CB | SER | 1154 | 73.331 | 58.483 | 57.903 | 1.00 | 40.16 |
| ATOM | 2059 | OG | SER | 1154 | 72.446 | 57.531 | 57.326 | 1.00 | 44.40 |
| ATOM | 2060 | C | SER | 1154 | 73.910 | 60.907 | 57.871 | 1.00 | 38.37 |
| ATOM | 2061 | O | SER | 1154 | 74.946 | 60.743 | 57.236 | 1.00 | 38.18 |
| ATOM | 2062 | N | PRO | 1155 | 73.694 | 62.005 | 58.622 | 1.00 | 38.99 |
| ATOM | 2063 | CD | PRO | 1155 | 72.505 | 62.296 | 59.437 | 1.00 | 39.19 |
| ATOM | 2064 | CA | PRO | 1155 | 74.708 | 63.045 | 58.805 | 1.00 | 38.38 |
| ATOM | 2065 | CB | PRO | 1155 | 74.098 | 63.942 | 59.875 | 1.00 | 38.04 |
| ATOM | 2066 | CG | PRO | 1155 | 73.120 | 63.040 | 60.584 | 1.00 | 40.36 |
| ATOM | 2067 | C | PRO | 1155 | 76.048 | 62.479 | 59.245 | 1.00 | 37.35 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM 2068 | O | PRO | 1155 | 76.121 | 61.531 | 60.044 | 1.00 | 36.59 |
| ATOM 2069 | N | ARG | 1156 | 77.104 | 63.088 | 58.732 | 1.00 | 36.29 |
| ATOM 2070 | CA | ARG | 1156 | 78.456 | 62.654 | 59.023 | 1.00 | 35.23 |
| ATOM 2071 | CB | ARG | 1156 | 79.031 | 61.956 | 57.803 | 1.00 | 38.13 |
| ATOM 2072 | CG | ARG | 1156 | 78.185 | 60.870 | 57.211 | 1.00 | 41.38 |
| ATOM 2073 | CD | ARG | 1156 | 78.700 | 59.509 | 57.644 | 1.00 | 44.77 |
| ATOM 2074 | NE | ARG | 1156 | 78.123 | 58.412 | 56.868 | 1.00 | 49.49 |
| ATOM 2075 | CZ | ARG | 1156 | 78.459 | 57.129 | 57.005 | 1.00 | 53.79 |
| ATOM 2076 | NH1 | ARG | 1156 | 77.873 | 56.205 | 56.252 | 1.00 | 54.43 |
| ATOM 2077 | NH2 | ARG | 1156 | 79.403 | 56.763 | 57.863 | 1.00 | 52.82 |
| ATOM 2078 | C | ARG | 1156 | 79.340 | 63.849 | 59.255 | 1.00 | 34.55 |
| ATOM 2079 | O | ARG | 1156 | 79.066 | 64.939 | 58.756 | 1.00 | 35.72 |
| ATOM 2080 | N | PRO | 1157 | 80.443 | 63.673 | 59.989 | 1.00 | 34.18 |
| ATOM 2081 | CD | PRO | 1157 | 80.899 | 62.473 | 60.707 | 1.00 | 33.27 |
| ATOM 2082 | CA | PRO | 1157 | 81.344 | 64.798 | 60.233 | 1.00 | 33.99 |
| ATOM 2083 | CB | PRO | 1157 | 82.419 | 64.167 | 61.111 | 1.00 | 33.27 |
| ATOM 2084 | CG | PRO | 1157 | 81.690 | 63.074 | 61.803 | 1.00 | 32.25 |
| ATOM 2085 | C | PRO | 1157 | 81.950 | 65.234 | 58.898 | 1.00 | 35.59 |
| ATOM 2086 | O | PRO | 1157 | 82.404 | 64.393 | 58.130 | 1.00 | 37.92 |
| ATOM 2087 | N | ILE | 1158 | 81.999 | 66.527 | 58.631 | 1.00 | 36.57 |
| ATOM 2088 | CA | ILE | 1158 | 82.542 | 67.000 | 57.362 | 1.00 | 38.10 |
| ATOM 2089 | CB | ILE | 1158 | 82.647 | 68.533 | 57.315 | 1.00 | 38.12 |
| ATOM 2090 | CG2 | ILE | 1158 | 81.272 | 69.140 | 57.171 | 1.00 | 37.34 |
| ATOM 2091 | CG1 | ILE | 1158 | 83.342 | 69.046 | 58.573 | 1.00 | 41.61 |
| ATOM 2092 | CD1 | ILE | 1158 | 83.623 | 70.540 | 58.559 | 1.00 | 45.60 |
| ATOM 2093 | C | ILE | 1158 | 83.911 | 66.408 | 57.004 | 1.00 | 39.96 |
| ATOM 2094 | O | ILE | 1158 | 84.280 | 66.367 | 55.828 | 1.00 | 41.17 |
| ATOM 2095 | N | SER | 1159 | 84.642 | 65.941 | 58.014 | 1.00 | 40.39 |
| ATOM 2096 | CA | SER | 1159 | 85.959 | 65.341 | 57.813 | 1.00 | 42.66 |
| ATOM 2097 | CB | SER | 1159 | 86.575 | 64.975 | 59.161 | 1.00 | 45.98 |
| ATOM 2098 | OG | SER | 1159 | 85.755 | 64.035 | 59.842 | 1.00 | 49.77 |
| ATOM 2099 | C | SER | 1159 | 85.870 | 64.078 | 56.955 | 1.00 | 42.30 |
| ATOM 2100 | O | SER | 1159 | 86.779 | 63.761 | 56.183 | 1.00 | 43.56 |
| ATOM 2101 | N | TYR | 1160 | 84.779 | 63.346 | 57.130 | 1.00 | 40.66 |
| ATOM 2102 | CA | TYR | 1160 | 84.531 | 62.121 | 56.385 | 1.00 | 40.36 |
| ATOM 2103 | CB | TYR | 1160 | 83.137 | 61.598 | 56.756 | 1.00 | 43.66 |
| ATOM 2104 | CG | TYR | 1160 | 82.848 | 60.149 | 56.423 | 1.00 | 47.75 |
| ATOM 2105 | CD1 | TYR | 1160 | 82.086 | 59.377 | 57.290 | 1.00 | 50.46 |
| ATOM 2106 | CE1 | TYR | 1160 | 81.763 | 58.059 | 56.991 | 1.00 | 53.68 |
| ATOM 2107 | CD2 | TYR | 1160 | 83.293 | 59.561 | 55.233 | 1.00 | 49.34 |
| ATOM 2108 | CE2 | TYR | 1160 | 82.975 | 58.237 | 54.922 | 1.00 | 51.68 |
| ATOM 2109 | CZ | TYR | 1160 | 82.205 | 57.493 | 55.809 | 1.00 | 53.15 |
| ATOM 2110 | OH | TYR | 1160 | 81.858 | 56.185 | 55.528 | 1.00 | 54.20 |
| ATOM 2111 | C | TYR | 1160 | 84.563 | 62.464 | 54.901 | 1.00 | 37.91 |
| ATOM 2112 | O | TYR | 1160 | 85.111 | 61.715 | 54.080 | 1.00 | 38.62 |
| ATOM 2113 | N | LEU | 1161 | 84.020 | 63.632 | 54.578 | 1.00 | 34.26 |
| ATOM 2114 | CA | LEU | 1161 | 83.932 | 64.086 | 53.203 | 1.00 | 30.68 |
| ATOM 2115 | CB | LEU | 1161 | 82.639 | 64.889 | 53.018 | 1.00 | 27.49 |
| ATOM 2116 | CG | LEU | 1161 | 81.344 | 64.152 | 53.394 | 1.00 | 25.85 |
| ATOM 2117 | CD1 | LEU | 1161 | 80.168 | 65.085 | 53.276 | 1.00 | 25.64 |
| ATOM 2118 | CD2 | LEU | 1161 | 81.135 | 62.931 | 52.516 | 1.00 | 23.54 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2119 | C | LEU | 1161 | 85.148 | 64.852 | 52.675 | 1.00 | 30.40 |
| ATOM | 2120 | O | LEU | 1161 | 85.242 | 65.106 | 51.473 | 1.00 | 31.18 |
| ATOM | 2121 | N | ALA | 1162 | 86.094 | 65.189 | 53.545 | 1.00 | 29.45 |
| ATOM | 2122 | CA | ALA | 1162 | 87.283 | 65.919 | 53.101 | 1.00 | 29.15 |
| ATOM | 2123 | CB | ALA | 1162 | 88.222 | 66.214 | 54.281 | 1.00 | 29.64 |
| ATOM | 2124 | C | ALA | 1162 | 88.024 | 65.140 | 52.015 | 1.00 | 27.83 |
| ATOM | 2125 | O | ALA | 1162 | 88.278 | 63.937 | 52.150 | 1.00 | 28.97 |
| ATOM | 2126 | N | GLY | 1163 | 88.324 | 65.830 | 50.922 | 1.00 | 26.09 |
| ATOM | 2127 | CA | GLY | 1163 | 89.032 | 65.216 | 49.816 | 1.00 | 24.79 |
| ATOM | 2128 | C | GLY | 1163 | 88.127 | 64.490 | 48.845 | 1.00 | 22.40 |
| ATOM | 2129 | O | GLY | 1163 | 88.607 | 63.799 | 47.958 | 1.00 | 22.88 |
| ATOM | 2130 | N | SER | 1164 | 86.819 | 64.667 | 48.978 | 1.00 | 23.08 |
| ATOM | 2131 | CA | SER | 1164 | 85.887 | 63.988 | 48.091 | 1.00 | 23.47 |
| ATOM | 2132 | CB | SER | 1164 | 84.765 | 63.336 | 48.893 | 1.00 | 22.44 |
| ATOM | 2133 | OG | SER | 1164 | 85.308 | 62.418 | 49.833 | 1.00 | 24.67 |
| ATOM | 2134 | C | SER | 1164 | 85.314 | 64.853 | 46.984 | 1.00 | 23.93 |
| ATOM | 2135 | O | SER | 1164 | 84.470 | 64.389 | 46.229 | 1.00 | 25.83 |
| ATOM | 2136 | N | SER | 1165 | 85.762 | 66.102 | 46.877 | 1.00 | 24.65 |
| ATOM | 2137 | CA | SER | 1165 | 85.271 | 66.981 | 45.815 | 1.00 | 24.90 |
| ATOM | 2138 | CB | SER | 1165 | 85.812 | 68.401 | 45.981 | 1.00 | 26.62 |
| ATOM | 2139 | OG | SER | 1165 | 85.674 | 68.850 | 47.316 | 1.00 | 33.09 |
| ATOM | 2140 | C | SER | 1165 | 85.756 | 66.423 | 44.487 | 1.00 | 22.54 |
| ATOM | 2141 | O | SER | 1165 | 86.942 | 66.152 | 44.327 | 1.00 | 22.12 |
| ATOM | 2142 | N | GLY | 1166 | 84.843 | 66.286 | 43.533 | 1.00 | 21.99 |
| ATOM | 2143 | CA | GLY | 1166 | 85.184 | 65.741 | 42.232 | 1.00 | 19.49 |
| ATOM | 2144 | C | GLY | 1166 | 84.745 | 64.288 | 42.122 | 1.00 | 20.47 |
| ATOM | 2145 | O | GLY | 1166 | 84.756 | 63.720 | 41.033 | 1.00 | 19.68 |
| ATOM | 2146 | N | GLY | 1167 | 84.388 | 63.684 | 43.258 | 1.00 | 20.15 |
| ATOM | 2147 | CA | GLY | 1167 | 83.928 | 62.303 | 43.294 | 1.00 | 20.19 |
| ATOM | 2148 | C | GLY | 1167 | 82.534 | 62.182 | 42.712 | 1.00 | 20.08 |
| ATOM | 2149 | O | GLY | 1167 | 81.798 | 63.161 | 42.698 | 1.00 | 21.88 |
| ATOM | 2150 | N | PRO | 1168 | 82.109 | 60.986 | 42.297 | 1.00 | 20.02 |
| ATOM | 2151 | CD | PRO | 1168 | 82.901 | 59.746 | 42.208 | 1.00 | 20.29 |
| ATOM | 2152 | CA | PRO | 1168 | 80.786 | 60.792 | 41.710 | 1.00 | 19.44 |
| ATOM | 2153 | CB | PRO | 1168 | 81.002 | 59.553 | 40.851 | 1.00 | 21.21 |
| ATOM | 2154 | CG | PRO | 1168 | 81.880 | 58.729 | 41.726 | 1.00 | 18.35 |
| ATOM | 2155 | C | PRO | 1168 | 79.578 | 60.595 | 42.611 | 1.00 | 19.51 |
| ATOM | 2156 | O | PRO | 1168 | 79.683 | 60.068 | 43.712 | 1.00 | 20.28 |
| ATOM | 2157 | N | LEU | 1169 | 78.427 | 61.050 | 42.123 | 1.00 | 19.50 |
| ATOM | 2158 | CA | LEU | 1169 | 77.149 | 60.852 | 42.798 | 1.00 | 20.76 |
| ATOM | 2159 | CB | LEU | 1169 | 76.376 | 62.152 | 42.977 | 1.00 | 18.93 |
| ATOM | 2160 | CG | LEU | 1169 | 76.583 | 62.721 | 44.372 | 1.00 | 17.23 |
| ATOM | 2161 | CD1 | LEU | 1169 | 77.483 | 63.924 | 44.272 | 1.00 | 17.53 |
| ATOM | 2162 | CD2 | LEU | 1169 | 75.255 | 63.072 | 44.991 | 1.00 | 16.81 |
| ATOM | 2163 | C | LEU | 1169 | 76.444 | 59.952 | 41.807 | 1.00 | 21.18 |
| ATOM | 2164 | O | LEU | 1169 | 76.098 | 60.381 | 40.708 | 1.00 | 23.71 |
| ATOM | 2165 | N | LEU | 1170 | 76.336 | 58.680 | 42.153 | 1.00 | 21.28 |
| ATOM | 2166 | CA | LEU | 1170 | 75.736 | 57.702 | 41.267 | 1.00 | 21.46 |
| ATOM | 2167 | CB | LEU | 1170 | 76.527 | 56.398 | 41.356 | 1.00 | 17.58 |
| ATOM | 2168 | CG | LEU | 1170 | 78.027 | 56.488 | 41.086 | 1.00 | 15.37 |
| ATOM | 2169 | CD1 | LEU | 1170 | 78.700 | 55.235 | 41.566 | 1.00 | 13.10 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2170 | CD2 | LEU | 1170 | 78.284 | 56.702 | 39.616 | 1.00 | 12.53 |
| ATOM | 2171 | C | LEU | 1170 | 74.265 | 57.416 | 41.529 | 1.00 | 24.11 |
| ATOM | 2172 | O | LEU | 1170 | 73.783 | 57.534 | 42.656 | 1.00 | 27.04 |
| ATOM | 2173 | N | CYS | 1171 | 73.540 | 57.104 | 40.466 | 1.00 | 23.89 |
| ATOM | 2174 | CA | CYS | 1171 | 72.142 | 56.747 | 40.592 | 1.00 | 26.02 |
| ATOM | 2175 | CB | CYS | 1171 | 71.421 | 56.978 | 39.265 | 1.00 | 26.82 |
| ATOM | 2176 | SG | CYS | 1171 | 71.658 | 55.657 | 38.066 | 1.00 | 28.93 |
| ATOM | 2177 | C | CYS | 1171 | 72.209 | 55.250 | 40.918 | 1.00 | 27.13 |
| ATOM | 2178 | O | CYS | 1171 | 73.285 | 54.648 | 40.840 | 1.00 | 28.91 |
| ATOM | 2179 | N | PRO | 1172 | 71.069 | 54.616 | 41.243 | 1.00 | 27.20 |
| ATOM | 2180 | CD | PRO | 1172 | 69.735 | 55.217 | 41.411 | 1.00 | 26.50 |
| ATOM | 2181 | CA | PRO | 1172 | 71.033 | 53.185 | 41.574 | 1.00 | 25.65 |
| ATOM | 2182 | CB | PRO | 1172 | 69.538 | 52.912 | 41.707 | 1.00 | 25.61 |
| ATOM | 2183 | CG | PRO | 1172 | 69.031 | 54.192 | 42.263 | 1.00 | 28.15 |
| ATOM | 2184 | C | PRO | 1172 | 71.681 | 52.239 | 40.558 | 1.00 | 25.57 |
| ATOM | 2185 | O | PRO | 1172 | 72.227 | 51.198 | 40.933 | 1.00 | 26.76 |
| ATOM | 2186 | N | ALA | 1173 | 71.606 | 52.576 | 39.277 | 1.00 | 25.34 |
| ATOM | 2187 | CA | ALA | 1173 | 72.193 | 51.729 | 38.244 | 1.00 | 25.38 |
| ATOM | 2188 | CB | ALA | 1173 | 71.454 | 51.915 | 36.936 | 1.00 | 25.17 |
| ATOM | 2189 | C | ALA | 1173 | 73.678 | 51.997 | 38.042 | 1.00 | 27.51 |
| ATOM | 2190 | O | ALA | 1173 | 74.279 | 51.483 | 37.095 | 1.00 | 29.05 |
| ATOM | 2191 | N | GLY | 1174 | 74.253 | 52.849 | 38.890 | 1.00 | 27.48 |
| ATOM | 2192 | CA | GLY | 1174 | 75.668 | 53.166 | 38.787 | 1.00 | 27.28 |
| ATOM | 2193 | C | GLY | 1174 | 76.035 | 54.129 | 37.673 | 1.00 | 26.52 |
| ATOM | 2194 | O | GLY | 1174 | 77.103 | 54.029 | 37.076 | 1.00 | 27.07 |
| ATOM | 2195 | N | HIS | 1175 | 75.140 | 55.047 | 37.353 | 1.00 | 25.55 |
| ATOM | 2196 | CA | HIS | 1175 | 75.427 | 56.016 | 36.312 | 1.00 | 25.00 |
| ATOM | 2197 | CB | HIS | 1175 | 74.313 | 56.027 | 35.281 | 1.00 | 26.94 |
| ATOM | 2198 | CG | HIS | 1175 | 74.268 | 54.783 | 34.458 | 1.00 | 27.86 |
| ATOM | 2199 | CD2 | HIS | 1175 | 74.317 | 54.598 | 33.121 | 1.00 | 30.29 |
| ATOM | 2200 | ND1 | HIS | 1175 | 74.228 | 53.525 | 35.018 | 1.00 | 30.38 |
| ATOM | 2201 | CE1 | HIS | 1175 | 74.254 | 52.616 | 34.061 | 1.00 | 31.15 |
| ATOM | 2202 | NE2 | HIS | 1175 | 74.310 | 53.241 | 32.900 | 1.00 | 31.52 |
| ATOM | 2203 | C | HIS | 1175 | 75.625 | 57.371 | 36.955 | 1.00 | 24.78 |
| ATOM | 2204 | O | HIS | 1175 | 75.027 | 57.656 | 37.990 | 1.00 | 27.48 |
| ATOM | 2205 | N | ALA | 1176 | 76.473 | 58.198 | 36.358 | 1.00 | 23.70 |
| ATOM | 2206 | CA | ALA | 1176 | 76.782 | 59.506 | 36.913 | 1.00 | 21.48 |
| ATOM | 2207 | CB | ALA | 1176 | 77.996 | 60.107 | 36.210 | 1.00 | 20.07 |
| ATOM | 2208 | C | ALA | 1176 | 75.630 | 60.492 | 36.910 | 1.00 | 21.16 |
| ATOM | 2209 | O | ALA | 1176 | 75.016 | 60.740 | 35.881 | 1.00 | 21.05 |
| ATOM | 2210 | N | VAL | 1177 | 75.339 | 61.036 | 38.083 | 1.00 | 20.47 |
| ATOM | 2211 | CA | VAL | 1177 | 74.286 | 62.025 | 38.254 | 1.00 | 20.12 |
| ATOM | 2212 | CB | VAL | 1177 | 73.375 | 61.663 | 39.454 | 1.00 | 22.63 |
| ATOM | 2213 | CG1 | VAL | 1177 | 72.432 | 62.818 | 39.789 | 1.00 | 21.63 |
| ATOM | 2214 | CG2 | VAL | 1177 | 72.574 | 60.399 | 39.141 | 1.00 | 20.84 |
| ATOM | 2215 | C | VAL | 1177 | 74.933 | 63.402 | 38.469 | 1.00 | 20.43 |
| ATOM | 2216 | O | VAL | 1177 | 74.374 | 64.436 | 38.086 | 1.00 | 19.45 |
| ATOM | 2217 | N | GLY | 1178 | 76.136 | 63.409 | 39.035 | 1.00 | 20.41 |
| ATOM | 2218 | CA | GLY | 1178 | 76.836 | 64.661 | 39.267 | 1.00 | 18.90 |
| ATOM | 2219 | C | GLY | 1178 | 78.153 | 64.429 | 39.972 | 1.00 | 18.98 |
| ATOM | 2220 | O | GLY | 1178 | 78.499 | 63.283 | 40.271 | 1.00 | 19.19 |

4/9/60

FIGURE 3 (CONT.)

| ATOM 2221 | N | LEU | 1179 | 78.887 | 65.508 | 40.230 | 1.00 | 18.30 |
|---|---|---|---|---|---|---|---|---|
| ATOM 2222 | CA | LEU | 1179 | 80.173 | 65.435 | 40.919 | 1.00 | 18.00 |
| ATOM 2223 | CB | LEU | 1179 | 81.298 | 66.027 | 40.054 | 1.00 | 12.80 |
| ATOM 2224 | CG | LEU | 1179 | 81.484 | 65.535 | 38.614 | 1.00 | 12.14 |
| ATOM 2225 | CD1 | LEU | 1179 | 82.733 | 66.154 | 38.040 | 1.00 | 9.04 |
| ATOM 2226 | CD2 | LEU | 1179 | 81.568 | 64.034 | 38.557 | 1.00 | 11.17 |
| ATOM 2227 | C | LEU | 1179 | 80.058 | 66.223 | 42.221 | 1.00 | 18.90 |
| ATOM 2228 | O | LEU | 1179 | 79.564 | 67.344 | 42.223 | 1.00 | 23.62 |
| ATOM 2229 | N | PHE | 1180 | 80.476 | 65.632 | 43.332 | 1.00 | 19.19 |
| ATOM 2230 | CA | PHE | 1180 | 80.418 | 66.301 | 44.625 | 1.00 | 19.90 |
| ATOM 2231 | CB | PHE | 1180 | 80.994 | 65.370 | 45.692 | 1.00 | 18.26 |
| ATOM 2232 | CG | PHE | 1180 | 81.071 | 65.968 | 47.070 | 1.00 | 18.11 |
| ATOM 2233 | CD1 | PHE | 1180 | 82.281 | 66.015 | 47.752 | 1.00 | 18.51 |
| ATOM 2234 | CD2 | PHE | 1180 | 79.936 | 66.426 | 47.714 | 1.00 | 18.19 |
| ATOM 2235 | CE1 | PHE | 1180 | 82.357 | 66.504 | 49.054 | 1.00 | 15.60 |
| ATOM 2236 | CE2 | PHE | 1180 | 80.013 | 66.916 | 49.020 | 1.00 | 18.73 |
| ATOM 2237 | CZ | PHE | 1180 | 81.226 | 66.951 | 49.683 | 1.00 | 14.64 |
| ATOM 2238 | C | PHE | 1180 | 81.225 | 67.594 | 44.552 | 1.00 | 21.74 |
| ATOM 2239 | O | PHE | 1180 | 82.397 | 67.565 | 44.195 | 1.00 | 23.00 |
| ATOM 2240 | N | ARG | 1181 | 80.583 | 68.727 | 44.826 | 1.00 | 24.80 |
| ATOM 2241 | CA | ARG | 1181 | 81.270 | 70.020 | 44.800 | 1.00 | 26.34 |
| ATOM 2242 | CB | ARG | 1181 | 80.427 | 71.116 | 44.144 | 1.00 | 26.66 |
| ATOM 2243 | CG | ARG | 1181 | 81.215 | 72.411 | 43.959 | 1.00 | 29.11 |
| ATOM 2244 | CD | ARG | 1181 | 80.365 | 73.532 | 43.425 | 1.00 | 33.23 |
| ATOM 2245 | NE | ARG | 1181 | 79.368 | 73.951 | 44.403 | 1.00 | 39.30 |
| ATOM 2246 | CZ | ARG | 1181 | 78.054 | 73.952 | 44.189 | 1.00 | 41.81 |
| ATOM 2247 | NH1 | ARG | 1181 | 77.559 | 73.555 | 43.020 | 1.00 | 42.79 |
| ATOM 2248 | NH2 | ARG | 1181 | 77.231 | 74.345 | 45.158 | 1.00 | 44.71 |
| ATOM 2249 | C | ARG | 1181 | 81.636 | 70.475 | 46.200 | 1.00 | 26.61 |
| ATOM 2250 | O | ARG | 1181 | 82.801 | 70.745 | 46.485 | 1.00 | 29.02 |
| ATOM 2251 | N | ALA | 1182 | 80.641 | 70.572 | 47.069 | 1.00 | 26.67 |
| ATOM 2252 | CA | ALA | 1182 | 80.892 | 71.008 | 48.426 | 1.00 | 27.49 |
| ATOM 2253 | CB | ALA | 1182 | 80.867 | 72.513 | 48.493 | 1.00 | 29.65 |
| ATOM 2254 | C | ALA | 1182 | 79.855 | 70.427 | 49.358 | 1.00 | 28.32 |
| ATOM 2255 | O | ALA | 1182 | 78.764 | 70.072 | 48.926 | 1.00 | 28.73 |
| ATOM 2256 | N | ALA | 1183 | 80.200 | 70.327 | 50.634 | 1.00 | 28.98 |
| ATOM 2257 | CA | ALA | 1183 | 79.281 | 69.787 | 51.622 | 1.00 | 32.58 |
| ATOM 2258 | CB | ALA | 1183 | 80.030 | 68.926 | 52.633 | 1.00 | 33.65 |
| ATOM 2259 | C | ALA | 1183 | 78.544 | 70.906 | 52.333 | 1.00 | 34.36 |
| ATOM 2260 | O | ALA | 1183 | 79.093 | 71.991 | 52.541 | 1.00 | 34.73 |
| ATOM 2261 | N | VAL | 1184 | 77.290 | 70.635 | 52.680 | 1.00 | 36.46 |
| ATOM 2262 | CA | VAL | 1184 | 76.437 | 71.577 | 53.388 | 1.00 | 37.51 |
| ATOM 2263 | CB | VAL | 1184 | 75.019 | 71.572 | 52.816 | 1.00 | 36.89 |
| ATOM 2264 | CG1 | VAL | 1184 | 74.119 | 72.441 | 53.663 | 1.00 | 36.81 |
| ATOM 2265 | CG2 | VAL | 1184 | 75.033 | 72.041 | 51.373 | 1.00 | 36.21 |
| ATOM 2266 | C | VAL | 1184 | 76.375 | 71.110 | 54.830 | 1.00 | 39.28 |
| ATOM 2267 | O | VAL | 1184 | 75.844 | 70.041 | 55.116 | 1.00 | 39.09 |
| ATOM 2268 | N | CYS | 1185 | 76.875 | 71.927 | 55.744 | 1.00 | 44.38 |
| ATOM 2269 | CA | CYS | 1185 | 76.895 | 71.546 | 57.148 | 1.00 | 48.30 |
| ATOM 2270 | CB | CYS | 1185 | 78.232 | 70.868 | 57.450 | 1.00 | 51.20 |
| ATOM 2271 | SG | CYS | 1185 | 79.678 | 71.835 | 56.911 | 1.00 | 61.55 |

| ATOM | 2272 | C | CYS | 1185 | 76.654 | 72.660 | 58.166 | 1.00 | 47.66 |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 2273 | O | CYS | 1185 | 76.474 | 73.830 | 57.821 | 1.00 | 48.84 |
| ATOM | 2274 | N | ALA | 1186 | 76.674 | 72.263 | 59.432 | 1.00 | 46.42 |
| ATOM | 2275 | CA | ALA | 1186 | 76.482 | 73.153 | 60.563 | 1.00 | 45.62 |
| ATOM | 2276 | CB | ALA | 1186 | 75.005 | 73.436 | 60.755 | 1.00 | 46.93 |
| ATOM | 2277 | C | ALA | 1186 | 77.026 | 72.370 | 61.748 | 1.00 | 45.29 |
| ATOM | 2278 | O | ALA | 1186 | 76.737 | 71.184 | 61.888 | 1.00 | 44.78 |
| ATOM | 2279 | N | ARG | 1187 | 77.857 | 73.014 | 62.563 | 1.00 | 44.52 |
| ATOM | 2280 | CA | ARG | 1187 | 78.468 | 72.364 | 63.726 | 1.00 | 43.45 |
| ATOM | 2281 | CB | ARG | 1187 | 77.415 | 71.680 | 64.617 | 1.00 | 45.37 |
| ATOM | 2282 | CG | ARG | 1187 | 76.904 | 72.544 | 65.761 | 1.00 | 46.88 |
| ATOM | 2283 | CD | ARG | 1187 | 76.224 | 73.789 | 65.243 | 1.00 | 49.61 |
| ATOM | 2284 | NE | ARG | 1187 | 76.134 | 74.839 | 66.250 | 1.00 | 49.41 |
| ATOM | 2285 | CZ | ARG | 1187 | 75.294 | 75.867 | 66.178 | 1.00 | 50.80 |
| ATOM | 2286 | NH1 | ARG | 1187 | 74.461 | 75.988 | 65.148 | 1.00 | 50.93 |
| ATOM | 2287 | NH2 | ARG | 1187 | 75.280 | 76.772 | 67.146 | 1.00 | 50.83 |
| ATOM | 2288 | C | ARG | 1187 | 79.510 | 71.347 | 63.290 | 1.00 | 41.49 |
| ATOM | 2289 | O | ARG | 1187 | 79.995 | 70.557 | 64.098 | 1.00 | 43.20 |
| ATOM | 2290 | N | GLY | 1188 | 79.879 | 71.389 | 62.015 | 1.00 | 38.92 |
| ATOM | 2291 | CA | GLY | 1188 | 80.864 | 70.451 | 61.515 | 1.00 | 36.42 |
| ATOM | 2292 | C | GLY | 1188 | 80.282 | 69.107 | 61.126 | 1.00 | 34.79 |
| ATOM | 2293 | O | GLY | 1188 | 81.029 | 68.157 | 60.914 | 1.00 | 37.40 |
| ATOM | 2294 | N | VAL | 1189 | 78.960 | 69.014 | 61.037 | 1.00 | 32.66 |
| ATOM | 2295 | CA | VAL | 1189 | 78.303 | 67.771 | 60.653 | 1.00 | 30.43 |
| ATOM | 2296 | CB | VAL | 1189 | 77.228 | 67.334 | 61.689 | 1.00 | 31.40 |
| ATOM | 2297 | CG1 | VAL | 1189 | 76.468 | 66.111 | 61.199 | 1.00 | 31.51 |
| ATOM | 2298 | CG2 | VAL | 1189 | 77.872 | 67.017 | 63.018 | 1.00 | 33.33 |
| ATOM | 2299 | C | VAL | 1189 | 77.628 | 68.016 | 59.311 | 1.00 | 31.53 |
| ATOM | 2300 | O | VAL | 1189 | 76.740 | 68.867 | 59.203 | 1.00 | 31.66 |
| ATOM | 2301 | N | ALA | 1190 | 78.101 | 67.315 | 58.285 | 1.00 | 30.61 |
| ATOM | 2302 | CA | ALA | 1190 | 77.567 | 67.420 | 56.932 | 1.00 | 29.84 |
| ATOM | 2303 | CB | ALA | 1190 | 78.511 | 66.754 | 55.956 | 1.00 | 29.82 |
| ATOM | 2304 | C | ALA | 1190 | 76.198 | 66.760 | 56.856 | 1.00 | 31.17 |
| ATOM | 2305 | O | ALA | 1190 | 76.073 | 65.552 | 57.075 | 1.00 | 33.60 |
| ATOM | 2306 | N | ALA | 1191 | 75.174 | 67.545 | 56.542 | 1.00 | 29.63 |
| ATOM | 2307 | CA | ALA | 1191 | 73.821 | 67.021 | 56.443 | 1.00 | 27.51 |
| ATOM | 2308 | CB | ALA | 1191 | 72.880 | 67.836 | 57.313 | 1.00 | 27.97 |
| ATOM | 2309 | C | ALA | 1191 | 73.334 | 66.997 | 55.000 | 1.00 | 28.18 |
| ATOM | 2310 | O | ALA | 1191 | 72.409 | 66.253 | 54.668 | 1.00 | 31.13 |
| ATOM | 2311 | N | ALA | 1192 | 73.962 | 67.793 | 54.138 | 1.00 | 26.71 |
| ATOM | 2312 | CA | ALA | 1192 | 73.594 | 67.853 | 52.721 | 1.00 | 24.73 |
| ATOM | 2313 | CB | ALA | 1192 | 72.674 | 69.024 | 52.449 | 1.00 | 25.63 |
| ATOM | 2314 | C | ALA | 1192 | 74.858 | 68.002 | 51.909 | 1.00 | 24.75 |
| ATOM | 2315 | O | ALA | 1192 | 75.935 | 68.200 | 52.473 | 1.00 | 23.68 |
| ATOM | 2316 | N | VAL | 1193 | 74.738 | 67.893 | 50.591 | 1.00 | 25.76 |
| ATOM | 2317 | CA | VAL | 1193 | 75.897 | 68.017 | 49.712 | 1.00 | 26.76 |
| ATOM | 2318 | CB | VAL | 1193 | 76.503 | 66.627 | 49.325 | 1.00 | 27.03 |
| ATOM | 2319 | CG1 | VAL | 1193 | 76.940 | 65.861 | 50.566 | 1.00 | 26.31 |
| ATOM | 2320 | CG2 | VAL | 1193 | 75.512 | 65.807 | 48.515 | 1.00 | 27.41 |
| ATOM | 2321 | C | VAL | 1193 | 75.569 | 68.756 | 48.425 | 1.00 | 27.01 |
| ATOM | 2322 | O | VAL | 1193 | 74.608 | 68.413 | 47.735 | 1.00 | 27.50 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2323 | N | ASP | 1194 | 76.333 | 69.807 | 48.146 | 1.00 | 26.41 |
| ATOM | 2324 | CA | ASP | 1194 | 76.180 | 70.587 | 46.926 | 1.00 | 27.71 |
| ATOM | 2325 | CB | ASP | 1194 | 76.750 | 71.995 | 47.109 | 1.00 | 30.91 |
| ATOM | 2326 | CG | ASP | 1194 | 75.836 | 72.906 | 47.907 | 1.00 | 34.47 |
| ATOM | 2327 | OD1 | ASP | 1194 | 76.335 | 73.953 | 48.389 | 1.00 | 36.98 |
| ATOM | 2328 | OD2 | ASP | 1194 | 74.626 | 72.590 | 48.041 | 1.00 | 35.44 |
| ATOM | 2329 | C | ASP | 1194 | 76.958 | 69.895 | 45.817 | 1.00 | 26.97 |
| ATOM | 2330 | O | ASP | 1194 | 78.163 | 69.650 | 45.964 | 1.00 | 26.74 |
| ATOM | 2331 | N | PHE | 1195 | 76.296 | 69.608 | 44.701 | 1.00 | 24.78 |
| ATOM | 2332 | CA | PHE | 1195 | 76.976 | 68.948 | 43.599 | 1.00 | 23.72 |
| ATOM | 2333 | CB | PHE | 1195 | 76.625 | 67.458 | 43.546 | 1.00 | 23.09 |
| ATOM | 2334 | CG | PHE | 1195 | 75.185 | 67.171 | 43.244 | 1.00 | 21.65 |
| ATOM | 2335 | CD1 | PHE | 1195 | 74.748 | 67.042 | 41.933 | 1.00 | 21.20 |
| ATOM | 2336 | CD2 | PHE | 1195 | 74.268 | 66.991 | 44.276 | 1.00 | 22.38 |
| ATOM | 2337 | CE1 | PHE | 1195 | 73.417 | 66.736 | 41.650 | 1.00 | 20.66 |
| ATOM | 2338 | CE2 | PHE | 1195 | 72.935 | 66.684 | 44.005 | 1.00 | 21.40 |
| ATOM | 2339 | CZ | PHE | 1195 | 72.510 | 66.556 | 42.689 | 1.00 | 21.45 |
| ATOM | 2340 | C | PHE | 1195 | 76.755 | 69.592 | 42.244 | 1.00 | 24.27 |
| ATOM | 2341 | O | PHE | 1195 | 75.898 | 70.452 | 42.076 | 1.00 | 26.48 |
| ATOM | 2342 | N | ILE | 1196 | 77.572 | 69.181 | 41.285 | 1.00 | 23.52 |
| ATOM | 2343 | CA | ILE | 1196 | 77.521 | 69.679 | 39.925 | 1.00 | 22.71 |
| ATOM | 2344 | CB | ILE | 1196 | 78.946 | 69.790 | 39.354 | 1.00 | 22.75 |
| ATOM | 2345 | CG2 | ILE | 1196 | 78.903 | 70.308 | 37.923 | 1.00 | 24.48 |
| ATOM | 2346 | CG1 | ILE | 1196 | 79.804 | 70.682 | 40.255 | 1.00 | 21.53 |
| ATOM | 2347 | CD1 | ILE | 1196 | 81.283 | 70.593 | 39.987 | 1.00 | 20.43 |
| ATOM | 2348 | C | ILE | 1196 | 76.753 | 68.658 | 39.090 | 1.00 | 24.50 |
| ATOM | 2349 | O | ILE | 1196 | 77.240 | 67.552 | 38.856 | 1.00 | 25.41 |
| ATOM | 2350 | N | PRO | 1197 | 75.525 | 68.993 | 38.666 | 1.00 | 24.80 |
| ATOM | 2351 | CD | PRO | 1197 | 74.778 | 70.230 | 38.940 | 1.00 | 24.02 |
| ATOM | 2352 | CA | PRO | 1197 | 74.718 | 68.076 | 37.858 | 1.00 | 24.02 |
| ATOM | 2353 | CB | PRO | 1197 | 73.466 | 68.900 | 37.571 | 1.00 | 21.87 |
| ATOM | 2354 | CG | PRO | 1197 | 73.360 | 69.780 | 38.748 | 1.00 | 21.74 |
| ATOM | 2355 | C | PRO | 1197 | 75.444 | 67.751 | 36.557 | 1.00 | 24.76 |
| ATOM | 2356 | O | PRO | 1197 | 76.143 | 68.606 | 36.011 | 1.00 | 25.57 |
| ATOM | 2357 | N | VAL | 1198 | 75.267 | 66.537 | 36.044 | 1.00 | 26.89 |
| ATOM | 2358 | CA | VAL | 1198 | 75.923 | 66.159 | 34.797 | 1.00 | 28.24 |
| ATOM | 2359 | CB | VAL | 1198 | 75.541 | 64.746 | 34.338 | 1.00 | 27.91 |
| ATOM | 2360 | CG1 | VAL | 1198 | 76.318 | 64.392 | 33.091 | 1.00 | 32.68 |
| ATOM | 2361 | CG2 | VAL | 1198 | 75.869 | 63.747 | 35.401 | 1.00 | 28.52 |
| ATOM | 2362 | C | VAL | 1198 | 75.583 | 67.148 | 33.684 | 1.00 | 29.68 |
| ATOM | 2363 | O | VAL | 1198 | 76.397 | 67.390 | 32.794 | 1.00 | 31.51 |
| ATOM | 2364 | N | ALA | 1199 | 74.394 | 67.741 | 33.754 | 1.00 | 30.96 |
| ATOM | 2365 | CA | ALA | 1199 | 73.954 | 68.718 | 32.759 | 1.00 | 28.72 |
| ATOM | 2366 | CB | ALA | 1199 | 72.610 | 69.294 | 33.157 | 1.00 | 30.86 |
| ATOM | 2367 | C | ALA | 1199 | 74.970 | 69.838 | 32.603 | 1.00 | 27.35 |
| ATOM | 2368 | O | ALA | 1199 | 75.193 | 70.346 | 31.503 | 1.00 | 27.43 |
| ATOM | 2369 | N | ASN | 1200 | 75.593 | 70.223 | 33.707 | 1.00 | 25.52 |
| ATOM | 2370 | CA | ASN | 1200 | 76.586 | 71.280 | 33.671 | 1.00 | 25.79 |
| ATOM | 2371 | CB | ASN | 1200 | 76.951 | 71.723 | 35.084 | 1.00 | 25.77 |
| ATOM | 2372 | CG | ASN | 1200 | 75.810 | 72.442 | 35.789 | 1.00 | 27.58 |
| ATOM | 2373 | OD1 | ASN | 1200 | 76.015 | 73.075 | 36.828 | 1.00 | 29.86 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2374 | ND2 | ASN | 1200 | 74.602 | 72.337 | 35.246 | 1.00 | 25.16 |
| ATOM | 2375 | C | ASN | 1200 | 77.828 | 70.842 | 32.907 | 1.00 | 26.50 |
| ATOM | 2376 | O | ASN | 1200 | 78.544 | 71.681 | 32.358 | 1.00 | 25.46 |
| ATOM | 2377 | N | LEU | 1201 | 78.063 | 69.531 | 32.844 | 1.00 | 27.79 |
| ATOM | 2378 | CA | LEU | 1201 | 79.213 | 68.977 | 32.125 | 1.00 | 27.44 |
| ATOM | 2379 | CB | LEU | 1201 | 79.400 | 67.488 | 32.437 | 1.00 | 27.76 |
| ATOM | 2380 | CG | LEU | 1201 | 79.560 | 67.059 | 33.897 | 1.00 | 27.52 |
| ATOM | 2381 | CD1 | LEU | 1201 | 79.793 | 65.564 | 33.955 | 1.00 | 28.46 |
| ATOM | 2382 | CD2 | LEU | 1201 | 80.703 | 67.790 | 34.548 | 1.00 | 24.26 |
| ATOM | 2383 | C | LEU | 1201 | 79.021 | 69.163 | 30.627 | 1.00 | 26.96 |
| ATOM | 2384 | O | LEU | 1201 | 79.891 | 69.694 | 29.946 | 1.00 | 26.74 |
| ATOM | 2385 | N | GLU | 1202 | 77.864 | 68.752 | 30.125 | 1.00 | 27.76 |
| ATOM | 2386 | CA | GLU | 1202 | 77.555 | 68.886 | 28.703 | 1.00 | 30.15 |
| ATOM | 2387 | CB | GLU | 1202 | 76.207 | 68.237 | 28.404 | 1.00 | 35.17 |
| ATOM | 2388 | CG | GLU | 1202 | 75.915 | 68.080 | 26.912 | 1.00 | 42.07 |
| ATOM | 2389 | CD | GLU | 1202 | 76.742 | 66.985 | 26.247 | 1.00 | 45.05 |
| ATOM | 2390 | OE1 | GLU | 1202 | 76.867 | 65.882 | 26.837 | 1.00 | 45.05 |
| ATOM | 2391 | OE2 | GLU | 1202 | 77.253 | 67.232 | 25.129 | 1.00 | 48.05 |
| ATOM | 2392 | C | GLU | 1202 | 77.530 | 70.362 | 28.311 | 1.00 | 27.55 |
| ATOM | 2393 | O | GLU | 1202 | 77.988 | 70.746 | 27.239 | 1.00 | 26.78 |
| ATOM | 2394 | N | THR | 1203 | 76.989 | 71.182 | 29.200 | 1.00 | 27.54 |
| ATOM | 2395 | CA | THR | 1203 | 76.916 | 72.618 | 28.997 | 1.00 | 28.52 |
| ATOM | 2396 | CB | THR | 1203 | 76.183 | 73.278 | 30.168 | 1.00 | 29.70 |
| ATOM | 2397 | OG1 | THR | 1203 | 74.814 | 72.848 | 30.179 | 1.00 | 31.63 |
| ATOM | 2398 | CG2 | THR | 1203 | 76.248 | 74.787 | 30.066 | 1.00 | 30.94 |
| ATOM | 2399 | C | THR | 1203 | 78.336 | 73.175 | 28.923 | 1.00 | 30.35 |
| ATOM | 2400 | O | THR | 1203 | 78.630 | 74.038 | 28.099 | 1.00 | 31.87 |
| ATOM | 2401 | N | THR | 1204 | 79.204 | 72.693 | 29.810 | 1.00 | 30.89 |
| ATOM | 2402 | CA | THR | 1204 | 80.597 | 73.126 | 29.839 | 1.00 | 30.06 |
| ATOM | 2403 | CB | THR | 1204 | 81.325 | 72.545 | 31.070 | 1.00 | 27.84 |
| ATOM | 2404 | OG1 | THR | 1204 | 80.789 | 73.148 | 32.254 | 1.00 | 28.92 |
| ATOM | 2405 | CG2 | THR | 1204 | 82.823 | 72.804 | 31.010 | 1.00 | 26.94 |
| ATOM | 2406 | C | THR | 1204 | 81.329 | 72.732 | 28.551 | 1.00 | 31.06 |
| ATOM | 2407 | O | THR | 1204 | 82.238 | 73.435 | 28.113 | 1.00 | 31.97 |
| ATOM | 2408 | N | MET | 1205 | 80.918 | 71.622 | 27.940 | 1.00 | 30.02 |
| ATOM | 2409 | CA | MET | 1205 | 81.545 | 71.155 | 26.710 | 1.00 | 29.36 |
| ATOM | 2410 | CB | MET | 1205 | 81.286 | 69.670 | 26.503 | 1.00 | 26.89 |
| ATOM | 2411 | CG | MET | 1205 | 81.846 | 68.816 | 27.605 | 1.00 | 26.79 |
| ATOM | 2412 | SD | MET | 1205 | 81.869 | 67.096 | 27.164 | 1.00 | 25.34 |
| ATOM | 2413 | CE | MET | 1205 | 80.165 | 66.684 | 27.336 | 1.00 | 26.80 |
| ATOM | 2414 | C | MET | 1205 | 81.101 | 71.927 | 25.480 | 1.00 | 30.12 |
| ATOM | 2415 | O | MET | 1205 | 81.795 | 71.910 | 24.463 | 1.00 | 31.11 |
| ATOM | 2416 | N | ARG | 1206 | 79.944 | 72.582 | 25.560 | 1.00 | 32.04 |
| ATOM | 2417 | CA | ARG | 1206 | 79.425 | 73.372 | 24.443 | 1.00 | 32.33 |
| ATOM | 2418 | CB | ARG | 1206 | 77.898 | 73.466 | 24.509 | 1.00 | 33.91 |
| ATOM | 2419 | CG | ARG | 1206 | 77.180 | 72.147 | 24.315 | 1.00 | 36.45 |
| ATOM | 2420 | CD | ARG | 1206 | 75.689 | 72.368 | 24.083 | 1.00 | 39.82 |
| ATOM | 2421 | NE | ARG | 1206 | 74.994 | 72.858 | 25.274 | 1.00 | 44.02 |
| ATOM | 2422 | CZ | ARG | 1206 | 74.337 | 72.082 | 26.140 | 1.00 | 44.21 |
| ATOM | 2423 | NH1 | ARG | 1206 | 74.272 | 70.767 | 25.962 | 1.00 | 41.77 |
| ATOM | 2424 | NH2 | ARG | 1206 | 73.760 | 72.623 | 27.207 | 1.00 | 44.77 |

| ATOM | 2425 | C | ARG | 1206 | 80.030 | 74.780 | 24.404 | 1.00 | 31.71 |
| ATOM | 2426 | O | ARG | 1206 | 80.163 | 75.405 | 25.487 | 1.00 | 33.75 |

### sNS4ACOORDINATES    (Complex B)

| | Atom Type | Resid | # | X | Y | Z | OCC | B | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2535 | CB | LYS | 1677 | 101.069 | 76.195 | 38.823 | 1.00 | 42.61 |
| ATOM | 2536 | CG | LYS | 1677 | 100.696 | 76.412 | 40.284 | 1.00 | 45.42 |
| ATOM | 2537 | CD | LYS | 1677 | 99.373 | 77.170 | 40.435 | 1.00 | 48.57 |
| ATOM | 2538 | CE | LYS | 1677 | 99.221 | 77.735 | 41.859 | 1.00 | 50.16 |
| ATOM | 2539 | NZ | LYS | 1677 | 97.898 | 78.400 | 42.112 | 1.00 | 51.22 |
| ATOM | 2540 | C | LYS | 1677 | 102.635 | 74.294 | 38.331 | 1.00 | 39.53 |
| ATOM | 2541 | O | LYS | 1677 | 102.747 | 73.868 | 37.171 | 1.00 | 39.44 |
| ATOM | 2542 | N | LYS | 1677 | 103.162 | 76.602 | 37.521 | 1.00 | 40.63 |
| ATOM | 2543 | CA | LYS | 1677 | 102.536 | 75.793 | 38.615 | 1.00 | 40.89 |
| ATOM | 2544 | N | GLY | 1678 | 102.595 | 73.497 | 39.393 | 1.00 | 37.81 |
| ATOM | 2545 | CA | GLY | 1678 | 102.708 | 72.057 | 39.240 | 1.00 | 34.76 |
| ATOM | 2546 | C | GLY | 1678 | 101.509 | 71.417 | 38.576 | 1.00 | 31.90 |
| ATOM | 2547 | O | GLY | 1678 | 100.461 | 72.045 | 38.430 | 1.00 | 31.54 |
| ATOM | 2548 | N | SER | 1679 | 101.684 | 70.181 | 38.126 | 1.00 | 28.52 |
| ATOM | 2549 | CA | SER | 1679 | 100.606 | 69.443 | 37.497 | 1.00 | 25.57 |
| ATOM | 2550 | CB | SER | 1679 | 101.167 | 68.417 | 36.506 | 1.00 | 26.14 |
| ATOM | 2551 | OG | SER | 1679 | 101.609 | 69.016 | 35.303 | 1.00 | 24.59 |
| ATOM | 2552 | C | SER | 1679 | 99.807 | 68.703 | 38.562 | 1.00 | 24.40 |
| ATOM | 2553 | O | SER | 1679 | 100.280 | 68.506 | 39.688 | 1.00 | 24.38 |
| ATOM | 2554 | N | VAL | 1680 | 98.574 | 68.346 | 38.219 | 1.00 | 23.52 |
| ATOM | 2555 | CA | VAL | 1680 | 97.724 | 67.576 | 39.106 | 1.00 | 21.39 |
| ATOM | 2556 | CB | VAL | 1680 | 96.252 | 67.694 | 38.697 | 1.00 | 21.22 |
| ATOM | 2557 | CG1 | VAL | 1680 | 95.392 | 66.728 | 39.493 | 1.00 | 19.38 |
| ATOM | 2558 | CG2 | VAL | 1680 | 95.784 | 69.112 | 38.932 | 1.00 | 21.01 |
| ATOM | 2559 | C | VAL | 1680 | 98.230 | 66.158 | 38.894 | 1.00 | 20.14 |
| ATOM | 2560 | O | VAL | 1680 | 98.478 | 65.754 | 37.754 | 1.00 | 18.28 |
| ATOM | 2561 | N | VAL | 1681 | 98.463 | 65.442 | 39.990 | 1.00 | 20.40 |
| ATOM | 2562 | CA | VAL | 1681 | 98.990 | 64.085 | 39.922 | 1.00 | 20.62 |
| ATOM | 2563 | CB | VAL | 1681 | 100.343 | 63.971 | 40.678 | 1.00 | 18.90 |
| ATOM | 2564 | CG1 | VAL | 1681 | 100.968 | 62.616 | 40.454 | 1.00 | 19.40 |
| ATOM | 2565 | CG2 | VAL | 1681 | 101.283 | 65.039 | 40.231 | 1.00 | 20.79 |
| ATOM | 2566 | C | VAL | 1681 | 98.050 | 63.055 | 40.522 | 1.00 | 21.25 |
| ATOM | 2567 | O | VAL | 1681 | 97.459 | 63.277 | 41.584 | 1.00 | 19.23 |
| ATOM | 2568 | N | ILE | 1682 | 97.956 | 61.910 | 39.850 | 1.00 | 22.25 |
| ATOM | 2569 | CA | ILE | 1682 | 97.134 | 60.795 | 40.304 | 1.00 | 22.27 |
| ATOM | 2570 | CB | ILE | 1682 | 96.791 | 59.853 | 39.125 | 1.00 | 18.88 |
| ATOM | 2571 | CG2 | ILE | 1682 | 96.052 | 58.633 | 39.627 | 1.00 | 19.14 |
| ATOM | 2572 | CG1 | ILE | 1682 | 95.940 | 60.597 | 38.094 | 1.00 | 17.33 |
| ATOM | 2573 | CD1 | ILE | 1682 | 95.611 | 59.800 | 36.862 | 1.00 | 14.03 |
| ATOM | 2574 | C | ILE | 1682 | 97.926 | 60.028 | 41.376 | 1.00 | 23.98 |
| ATOM | 2575 | O | ILE | 1682 | 98.998 | 59.474 | 41.090 | 1.00 | 24.49 |
| ATOM | 2576 | N | VAL | 1683 | 97.425 | 60.045 | 42.611 | 1.00 | 24.04 |
| ATOM | 2577 | CA | VAL | 1683 | 98.074 | 59.345 | 43.724 | 1.00 | 22.87 |

FIGURE 3 (CONT.)

| ATOM | 2578 | CB | VAL | 1683 | 98.294 | 60.273 | 44.960 | 1.00 | 20.49 |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2579 | CG1 | VAL | 1683 | 99.218 | 61.422 | 44.602 | 1.00 | 21.14 |
| ATOM | 2580 | CG2 | VAL | 1683 | 96.986 | 60.787 | 45.493 | 1.00 | 15.48 |
| ATOM | 2581 | C | VAL | 1683 | 97.319 | 58.086 | 44.177 | 1.00 | 22.99 |
| ATOM | 2582 | O | VAL | 1683 | 97.667 | 57.470 | 45.190 | 1.00 | 25.32 |
| ATOM | 2583 | N | GLY | 1684 | 96.294 | 57.704 | 43.423 | 1.00 | 22.53 |
| ATOM | 2584 | CA | GLY | 1684 | 95.515 | 56.527 | 43.757 | 1.00 | 21.02 |
| ATOM | 2585 | C | GLY | 1684 | 94.291 | 56.452 | 42.870 | 1.00 | 21.67 |
| ATOM | 2586 | O | GLY | 1684 | 94.144 | 57.267 | 41.956 | 1.00 | 21.86 |
| ATOM | 2587 | N | ARG | 1685 | 93.399 | 55.507 | 43.154 | 1.00 | 22.35 |
| ATOM | 2588 | CA | ARG | 1685 | 92.177 | 55.327 | 42.369 | 1.00 | 19.90 |
| ATOM | 2589 | CB | ARG | 1685 | 92.449 | 54.463 | 41.150 | 1.00 | 20.04 |
| ATOM | 2590 | CG | ARG | 1685 | 93.003 | 53.105 | 41.516 | 1.00 | 22.48 |
| ATOM | 2591 | CD | ARG | 1685 | 93.157 | 52.240 | 40.296 | 1.00 | 26.67 |
| ATOM | 2592 | NE | ARG | 1685 | 94.237 | 51.271 | 40.446 | 1.00 | 28.97 |
| ATOM | 2593 | CZ | ARG | 1685 | 95.485 | 51.487 | 40.048 | 1.00 | 27.79 |
| ATOM | 2594 | NH1 | ARG | 1685 | 95.815 | 52.632 | 39.474 | 1.00 | 27.86 |
| ATOM | 2595 | NH2 | ARG | 1685 | 96.404 | 50.557 | 40.224 | 1.00 | 29.00 |
| ATOM | 2596 | C | ARG | 1685 | 91.113 | 54.636 | 43.185 | 1.00 | 20.01 |
| ATOM | 2597 | O | ARG | 1685 | 91.404 | 54.035 | 44.218 | 1.00 | 22.88 |
| ATOM | 2598 | N | ILE | 1686 | 89.882 | 54.703 | 42.697 | 1.00 | 18.51 |
| ATOM | 2599 | CA | ILE | 1686 | 88.745 | 54.066 | 43.346 | 1.00 | 17.38 |
| ATOM | 2600 | CB | ILE | 1686 | 87.823 | 55.120 | 43.985 | 1.00 | 15.63 |
| ATOM | 2601 | CG2 | ILE | 1686 | 86.464 | 54.533 | 44.292 | 1.00 | 14.38 |
| ATOM | 2602 | CG1 | ILE | 1686 | 88.496 | 55.665 | 45.251 | 1.00 | 14.48 |
| ATOM | 2603 | CD1 | ILE | 1686 | 87.740 | 56.758 | 45.935 | 1.00 | 14.17 |
| ATOM | 2604 | C | ILE | 1686 | 88.043 | 53.247 | 42.268 | 1.00 | 17.71 |
| ATOM | 2605 | O | ILE | 1686 | 87.699 | 53.769 | 41.205 | 1.00 | 17.73 |
| ATOM | 2606 | N | VAL | 1687 | 87.945 | 51.940 | 42.484 | 1.00 | 16.52 |
| ATOM | 2607 | CA | VAL | 1687 | 87.325 | 51.073 | 41.493 | 1.00 | 14.59 |
| ATOM | 2608 | CB | VAL | 1687 | 88.152 | 49.810 | 41.237 | 1.00 | 13.39 |
| ATOM | 2609 | CG1 | VAL | 1687 | 87.509 | 48.980 | 40.145 | 1.00 | 11.21 |
| ATOM | 2610 | CG2 | VAL | 1687 | 89.564 | 50.184 | 40.842 | 1.00 | 11.10 |
| ATOM | 2611 | C | VAL | 1687 | 85.922 | 50.681 | 41.874 | 1.00 | 15.40 |
| ATOM | 2612 | O | VAL | 1687 | 85.695 | 50.067 | 42.916 | 1.00 | 17.30 |
| ATOM | 2613 | N | LEU | 1688 | 84.990 | 51.081 | 41.016 | 1.00 | 16.16 |
| ATOM | 2614 | CA | LEU | 1688 | 83.566 | 50.827 | 41.171 | 1.00 | 15.94 |
| ATOM | 2615 | CB | LEU | 1688 | 82.792 | 52.003 | 40.578 | 1.00 | 14.08 |
| ATOM | 2616 | CG | LEU | 1688 | 82.936 | 53.300 | 41.365 | 1.00 | 15.70 |
| ATOM | 2617 | CD1 | LEU | 1688 | 82.611 | 54.511 | 40.519 | 1.00 | 15.92 |
| ATOM | 2618 | CD2 | LEU | 1688 | 82.026 | 53.212 | 42.559 | 1.00 | 18.17 |
| ATOM | 2619 | C | LEU | 1688 | 83.129 | 49.532 | 40.481 | 1.00 | 17.97 |
| ATOM | 2620 | O | LEU | 1688 | 82.209 | 48.856 | 40.939 | 1.00 | 20.09 |
| ATOM | 2621 | N | SER | 1689 | 83.826 | 49.174 | 39.406 | 1.00 | 20.02 |
| ATOM | 2622 | CA | SER | 1689 | 83.518 | 47.982 | 38.611 | 1.00 | 21.75 |
| ATOM | 2623 | CB | SER | 1689 | 84.253 | 48.060 | 37.266 | 1.00 | 23.96 |
| ATOM | 2624 | OG | SER | 1689 | 85.605 | 48.467 | 37.436 | 1.00 | 27.29 |
| ATOM | 2625 | C | SER | 1689 | 83.749 | 46.603 | 39.243 | 1.00 | 21.43 |
| ATOM | 2626 | O | SER | 1689 | 83.290 | 45.596 | 38.700 | 1.00 | 23.26 |
| ATOM | 2627 | N | GLY | 1690 | 84.465 | 46.547 | 40.364 | 1.00 | 21.24 |
| ATOM | 2628 | CA | GLY | 1690 | 84.724 | 45.277 | 41.015 | 1.00 | 19.68 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM 2629 | C | GLY | 1690 | 83.431 | 44.657 | 41.500 | 1.00 | 21.01 |
| ATOM 2630 | O | GLY | 1690 | 82.452 | 45.367 | 41.741 | 1.00 | 20.02 |
| ATOM 2631 | N | LYS | 1691 | 83.419 | 43.334 | 41.618 | 1.00 | 22.40 |
| ATOM 2632 | CA | LYS | 1691 | 82.245 | 42.596 | 42.075 | 1.00 | 25.78 |
| ATOM 2633 | CB | LYS | 1691 | 81.621 | 41.838 | 40.901 | 1.00 | 30.22 |
| ATOM 2634 | CG | LYS | 1691 | 81.068 | 42.740 | 39.813 | 1.00 | 38.96 |
| ATOM 2635 | CD | LYS | 1691 | 80.651 | 41.947 | 38.575 | 1.00 | 46.14 |
| ATOM 2636 | CE | LYS | 1691 | 80.270 | 42.880 | 37.405 | 1.00 | 49.42 |
| ATOM 2637 | NZ | LYS | 1691 | 79.814 | 42.127 | 36.186 | 1.00 | 50.87 |
| ATOM 2638 | C | LYS | 1691 | 82.705 | 41.610 | 43.142 | 1.00 | 25.02 |
| ATOM 2639 | O | LYS | 1691 | 83.885 | 41.254 | 43.176 | 1.00 | 26.26 |
| ATOM 2640 | N | PRO | 1692 | 81.796 | 41.167 | 44.031 | 1.00 | 23.86 |
| ATOM 2641 | CD | PRO | 1692 | 80.365 | 41.516 | 44.115 | 1.00 | 25.36 |
| ATOM 2642 | CA | PRO | 1692 | 82.157 | 40.217 | 45.088 | 1.00 | 23.51 |
| ATOM 2643 | CB | PRO | 1692 | 80.801 | 39.691 | 45.542 | 1.00 | 23.49 |
| ATOM 2644 | CG | PRO | 1692 | 79.954 | 40.911 | 45.451 | 1.00 | 24.91 |
| ATOM 2645 | C | PRO | 1692 | 83.027 | 39.095 | 44.548 | 1.00 | 23.24 |
| ATOM 2646 | O | PRO | 1692 | 82.724 | 38.506 | 43.515 | 1.00 | 25.88 |
| ATOM 2647 | N | ALA | 1693 | 84.136 | 38.831 | 45.219 | 1.00 | 21.89 |
| ATOM 2648 | CA | ALA | 1693 | 85.035 | 37.787 | 44.780 | 1.00 | 21.26 |
| ATOM 2649 | CB | ALA | 1693 | 86.173 | 38.383 | 43.989 | 1.00 | 21.74 |
| ATOM 2650 | C | ALA | 1693 | 85.568 | 37.089 | 46.000 | 1.00 | 22.42 |
| ATOM 2651 | O | ALA | 1693 | 85.708 | 37.705 | 47.055 | 1.00 | 24.98 |
| ATOM 2652 | N | ILE | 1694 | 85.810 | 35.791 | 45.879 | 1.00 | 22.49 |
| ATOM 2653 | CA | ILE | 1694 | 86.342 | 35.020 | 46.989 | 1.00 | 21.65 |
| ATOM 2654 | CB | ILE | 1694 | 86.052 | 33.524 | 46.794 | 1.00 | 20.10 |
| ATOM 2655 | CG2 | ILE | 1694 | 86.718 | 32.714 | 47.873 | 1.00 | 22.22 |
| ATOM 2656 | CG1 | ILE | 1694 | 84.539 | 33.293 | 46.829 | 1.00 | 20.16 |
| ATOM 2657 | CD1 | ILE | 1694 | 84.133 | 31.872 | 46.593 | 1.00 | 19.23 |
| ATOM 2658 | C | ILE | 1694 | 87.832 | 35.311 | 46.999 | 1.00 | 22.06 |
| ATOM 2659 | O | ILE | 1694 | 88.506 | 35.118 | 45.988 | 1.00 | 25.81 |
| ATOM 2660 | N | ILE | 1695 | 88.336 | 35.837 | 48.109 | 1.00 | 21.38 |
| ATOM 2661 | CA | ILE | 1695 | 89.748 | 36.181 | 48.194 | 1.00 | 19.73 |
| ATOM 2662 | CB | ILE | 1695 | 90.112 | 36.812 | 49.557 | 1.00 | 16.79 |
| ATOM 2663 | CG2 | ILE | 1695 | 91.550 | 37.296 | 49.533 | 1.00 | 16.53 |
| ATOM 2664 | CG1 | ILE | 1695 | 89.209 | 38.009 | 49.853 | 1.00 | 11.03 |
| ATOM 2665 | CD1 | ILE | 1695 | 89.480 | 38.658 | 51.192 | 1.00 | 8.12 |
| ATOM 2666 | C | ILE | 1695 | 90.596 | 34.943 | 47.947 | 1.00 | 22.82 |
| ATOM 2667 | O | ILE | 1695 | 90.498 | 33.954 | 48.669 | 1.00 | 22.97 |
| ATOM 2668 | N | PRO | 1696 | 91.407 | 34.967 | 46.886 | 1.00 | 26.75 |
| ATOM 2669 | CD | PRO | 1696 | 91.564 | 36.085 | 45.940 | 1.00 | 28.08 |
| ATOM 2670 | CA | PRO | 1696 | 92.279 | 33.851 | 46.520 | 1.00 | 30.50 |
| ATOM 2671 | CB | PRO | 1696 | 93.080 | 34.418 | 45.354 | 1.00 | 29.24 |
| ATOM 2672 | CG | PRO | 1696 | 92.138 | 35.395 | 44.733 | 1.00 | 28.73 |
| ATOM 2673 | C | PRO | 1696 | 93.207 | 33.490 | 47.662 | 1.00 | 36.92 |
| ATOM 2674 | O | PRO | 1696 | 93.659 | 34.371 | 48.402 | 1.00 | 37.43 |
| ATOM 2675 | N | LYS | 1697 | 93.454 | 32.191 | 47.824 | 1.00 | 42.85 |
| ATOM 2676 | CA | LYS | 1697 | 94.356 | 31.692 | 48.863 | 1.00 | 46.97 |
| ATOM 2677 | CB | LYS | 1697 | 93.938 | 30.284 | 49.314 | 1.00 | 48.62 |
| ATOM 2678 | CG | LYS | 1697 | 92.480 | 30.143 | 49.712 | 1.00 | 52.72 |
| ATOM 2679 | CD | LYS | 1697 | 92.325 | 29.631 | 51.139 | 1.00 | 54.54 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2680 | CE | LYS | 1697 | 90.885 | 29.167 | 51.394 | 1.00 | 56.49 |
| ATOM | 2681 | NZ | LYS | 1697 | 90.578 | 27.847 | 50.749 | 1.00 | 59.20 |
| ATOM | 2682 | C | LYS | 1697 | 95.789 | 31.645 | 48.311 | 1.00 | 48.94 |
| ATOM | 2683 | O | LYS | 1697 | 96.588 | 32.540 | 48.661 | 1.00 | 50.95 |

## ZINC ION COORDINATES

| | | Atom Type | Resid | # | X | Y | Z | OCC | B | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2684 | ZN | ZN | 901 | 71.089 | 51.399 | 51.975 | 1.00 | 29.52 |
| ATOM | 2685 | ZN | ZN | 902 | 70.157 | 56.302 | 36.264 | 1.00 | 32.22 |

## WATERMOLECULE COORDINATES

| | | Atom Type | Resid | # | X | Y | Z | OCC | B | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2686 | OH2 | TIP3 | 1 | 80.188 | 51.569 | 51.895 | 1.00 | 14.91 |
| ATOM | 2687 | OH2 | TIP3 | 2 | 84.436 | 50.278 | 50.706 | 1.00 | 27.51 |
| ATOM | 2688 | OH2 | TIP3 | 3 | 80.360 | 48.626 | 54.069 | 1.00 | 26.47 |
| ATOM | 2689 | OH2 | TIP3 | 4 | 90.933 | 33.696 | 52.289 | 1.00 | 23.43 |
| ATOM | 2690 | OH2 | TIP3 | 5 | 72.460 | 27.233 | 53.507 | 1.00 | 26.41 |
| ATOM | 2691 | OH2 | TIP3 | 6 | 87.098 | 37.167 | 56.456 | 1.00 | 35.13 |
| ATOM | 2692 | OH2 | TIP3 | 7 | 80.196 | 47.990 | 42.389 | 1.00 | 32.46 |
| ATOM | 2693 | OH2 | TIP3 | 8 | 80.634 | 37.946 | 41.797 | 1.00 | 15.54 |
| ATOM | 2694 | OH2 | TIP3 | 9 | 91.083 | 45.806 | 52.787 | 1.00 | 17.30 |
| ATOM | 2695 | OH2 | TIP3 | 10 | 85.712 | 53.247 | 29.331 | 1.00 | 28.74 |
| ATOM | 2696 | OH2 | TIP3 | 11 | 89.054 | 50.366 | 50.031 | 1.00 | 18.47 |
| ATOM | 2697 | OH2 | TIP3 | 12 | 79.767 | 46.999 | 50.439 | 1.00 | 24.04 |
| ATOM | 2698 | OH2 | TIP3 | 13 | 79.409 | 63.138 | 26.964 | 1.00 | 33.09 |
| ATOM | 2699 | OH2 | TIP3 | 14 | 79.565 | 49.986 | 49.688 | 1.00 | 26.32 |
| ATOM | 2700 | OH2 | TIP3 | 15 | 88.908 | 25.285 | 68.030 | 1.00 | 19.71 |
| ATOM | 2701 | OH2 | TIP3 | 16 | 59.074 | 46.155 | 52.416 | 1.00 | 29.76 |
| ATOM | 2702 | OH2 | TIP3 | 17 | 83.621 | 37.213 | 41.479 | 1.00 | 44.52 |
| ATOM | 2703 | OH2 | TIP3 | 18 | 59.694 | 46.148 | 55.800 | 1.00 | 34.49 |
| ATOM | 2704 | OH2 | TIP3 | 19 | 94.223 | 75.564 | 42.730 | 1.00 | 38.61 |
| ATOM | 2705 | OH2 | TIP3 | 20 | 66.565 | 41.471 | 68.855 | 1.00 | 40.67 |
| ATOM | 2706 | OH2 | TIP3 | 21 | 94.230 | 39.125 | 44.532 | 1.00 | 37.61 |
| ATOM | 2707 | OH2 | TIP3 | 22 | 63.801 | 32.294 | 63.606 | 1.00 | 24.75 |
| ATOM | 2708 | OH2 | TIP3 | 23 | 85.565 | 24.399 | 71.908 | 1.00 | 34.81 |
| ATOM | 2709 | OH2 | TIP3 | 24 | 78.876 | 64.139 | 29.678 | 1.00 | 39.51 |
| ATOM | 2710 | OH2 | TIP3 | 25 | 82.850 | 28.849 | 47.546 | 1.00 | 25.28 |
| ATOM | 2711 | OH2 | TIP3 | 28 | 69.172 | 69.500 | 51.903 | 1.00 | 30.62 |
| ATOM | 2712 | OH2 | TIP3 | 29 | 66.988 | 51.499 | 56.187 | 1.00 | 30.20 |
| ATOM | 2713 | OH2 | TIP3 | 30 | 91.719 | 42.057 | 60.299 | 1.00 | 31.11 |
| ATOM | 2714 | OH2 | TIP3 | 31 | 77.543 | 29.196 | 41.350 | 1.00 | 55.87 |
| ATOM | 2715 | OH2 | TIP3 | 32 | 84.613 | 22.791 | 54.244 | 1.00 | 64.87 |
| ATOM | 2716 | OH2 | TIP3 | 33 | 71.143 | 49.227 | 43.011 | 1.00 | 36.07 |
| ATOM | 2717 | OH2 | TIP3 | 34 | 72.527 | 52.824 | 53.213 | 1.00 | 5.56 |
| ATOM | 2718 | OH2 | TIP3 | 35 | 80.116 | 46.082 | 38.809 | 1.00 | 44.35 |

FIGURE 3 (CONT.)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2719 | OH2 | TIP3 | 36 | 65.304 | 58.306 | 50.404 | 1.00 | 50.48 |
| ATOM | 2720 | OH2 | TIP3 | 38 | 77.283 | 35.181 | 38.894 | 1.00 | 36.34 |
| ATOM | 2721 | OH2 | TIP3 | 39 | 67.275 | 62.937 | 39.441 | 1.00 | 39.30 |
| ATOM | 2722 | OH2 | TIP3 | 40 | 95.912 | 77.587 | 39.202 | 1.00 | 37.03 |
| ATOM | 2723 | OH2 | TIP3 | 41 | 87.028 | 46.815 | 50.178 | 1.00 | 14.09 |
| ATOM | 2724 | OH2 | TIP3 | 42 | 70.710 | 55.468 | 34.204 | 1.00 | 7.82 |
| ATOM | 2725 | OH2 | TIP3 | 43 | 87.279 | 67.965 | 49.287 | 1.00 | 23.95 |
| ATOM | 2726 | OH2 | TIP3 | 44 | 90.719 | 39.572 | 46.110 | 1.00 | 29.46 |
| ATOM | 2727 | OH2 | TIP3 | 45 | 88.956 | 32.992 | 50.562 | 1.00 | 26.01 |
| ATOM | 2728 | OH2 | TIP3 | 46 | 99.309 | 29.693 | 67.462 | 1.00 | 19.97 |
| ATOM | 2729 | OH2 | TIP3 | 47 | 99.173 | 61.794 | 37.290 | 1.00 | 31.61 |
| ATOM | 2730 | OH2 | TIP3 | 48 | 106.963 | 58.636 | 47.340 | 1.00 | 36.68 |
| ATOM | 2731 | OH2 | TIP3 | 49 | 85.142 | 35.133 | 43.034 | 1.00 | 19.23 |
| ATOM | 2732 | OH2 | TIP3 | 50 | 71.616 | 67.146 | 35.073 | 1.00 | 36.90 |
| ATOM | 2733 | OH2 | TIP3 | 51 | 75.865 | 23.589 | 68.938 | 1.00 | 31.60 |
| ATOM | 2734 | OH2 | TIP3 | 52 | 84.026 | 47.614 | 42.760 | 1.00 | 26.85 |
| ATOM | 2735 | OH2 | TIP3 | 53 | 99.401 | 56.479 | 39.758 | 1.00 | 21.95 |
| ATOM | 2736 | OH2 | TIP3 | 54 | 68.040 | 27.725 | 53.497 | 1.00 | 43.99 |
| ATOM | 2737 | OH2 | TIP3 | 55 | 78.583 | 39.197 | 40.332 | 1.00 | 24.68 |
| ATOM | 2738 | OH2 | TIP3 | 56 | 92.451 | 75.069 | 27.711 | 1.00 | 44.43 |
| ATOM | 2739 | OH2 | TIP3 | 57 | 89.623 | 49.854 | 35.111 | 1.00 | 22.90 |
| ATOM | 2740 | OH2 | TIP3 | 58 | 95.616 | 73.094 | 31.597 | 1.00 | 27.62 |
| ATOM | 2741 | OH2 | TIP3 | 59 | 86.253 | 47.246 | 59.568 | 1.00 | 24.37 |
| ATOM | 2742 | OH2 | TIP3 | 60 | 98.881 | 56.884 | 37.033 | 1.00 | 32.28 |
| ATOM | 2743 | OH2 | TIP3 | 61 | 107.913 | 59.670 | 50.434 | 1.00 | 40.73 |
| ATOM | 2744 | OH2 | TIP3 | 62 | 63.410 | 58.104 | 43.219 | 1.00 | 29.77 |
| ATOM | 2745 | OH2 | TIP3 | 63 | 99.184 | 62.943 | 48.341 | 1.00 | 52.93 |
| ATOM | 2746 | OH2 | TIP3 | 64 | 92.483 | 47.893 | 40.686 | 1.00 | 33.31 |
| ATOM | 2747 | OH2 | TIP3 | 65 | 76.471 | 22.799 | 61.366 | 1.00 | 33.07 |
| ATOM | 2748 | OH2 | TIP3 | 66 | 102.733 | 70.701 | 43.239 | 1.00 | 52.51 |
| ATOM | 2749 | OH2 | TIP3 | 67 | 94.669 | 46.032 | 46.815 | 1.00 | 31.75 |
| ATOM | 2750 | OH2 | TIP3 | 68 | 100.962 | 67.281 | 48.137 | 1.00 | 52.13 |
| ATOM | 2751 | OH2 | TIP3 | 69 | 76.478 | 37.405 | 40.145 | 1.00 | 25.79 |
| ATOM | 2752 | OH2 | TIP3 | 70 | 90.165 | 47.004 | 58.770 | 1.00 | 49.51 |
| ATOM | 2753 | OH2 | TIP3 | 71 | 89.912 | 38.696 | 43.283 | 1.00 | 41.39 |
| ATOM | 2754 | OH2 | TIP3 | 72 | 78.867 | 77.910 | 30.979 | 1.00 | 43.29 |
| ATOM | 2755 | OH2 | TIP3 | 73 | 105.807 | 71.061 | 33.955 | 1.00 | 35.91 |
| ATOM | 2756 | OH2 | TIP3 | 74 | 94.956 | 46.168 | 41.472 | 1.00 | 32.83 |
| ATOM | 2757 | OH2 | TIP3 | 75 | 81.755 | 20.284 | 64.565 | 1.00 | 36.36 |
| ATOM | 2758 | OH2 | TIP3 | 76 | 83.777 | 36.376 | 73.095 | 1.00 | 35.68 |
| ATOM | 2759 | OH2 | TIP3 | 77 | 90.384 | 42.253 | 62.669 | 1.00 | 45.35 |
| ATOM | 2760 | OH2 | TIP3 | 78 | 88.037 | 29.259 | 75.147 | 1.00 | 56.66 |
| ATOM | 2761 | OH2 | TIP3 | 79 | 101.859 | 65.470 | 26.683 | 1.00 | 39.64 |
| ATOM | 2762 | OH2 | TIP3 | 80 | 71.347 | 27.770 | 73.090 | 1.00 | 46.49 |
| ATOM | 2763 | OH2 | TIP3 | 81 | 105.055 | 72.336 | 36.481 | 1.00 | 34.57 |
| ATOM | 2764 | OH2 | TIP3 | 82 | 89.487 | 32.603 | 43.952 | 1.00 | 55.98 |
| ATOM | 2765 | OH2 | TIP3 | 83 | 82.955 | 70.726 | 51.485 | 1.00 | 31.53 |
| ATOM | 2766 | OH2 | TIP3 | 84 | 104.149 | 69.529 | 35.834 | 1.00 | 22.24 |
| ATOM | 2767 | OH2 | TIP3 | 87 | 97.144 | 58.485 | 29.113 | 1.00 | 38.50 |
| ATOM | 2768 | OH2 | TIP3 | 88 | 99.143 | 58.146 | 34.137 | 1.00 | 31.08 |
| ATOM | 2769 | OH2 | TIP3 | 89 | 93.402 | 76.905 | 45.088 | 1.00 | 58.17 |

## FIGURE 3 (CONT.)

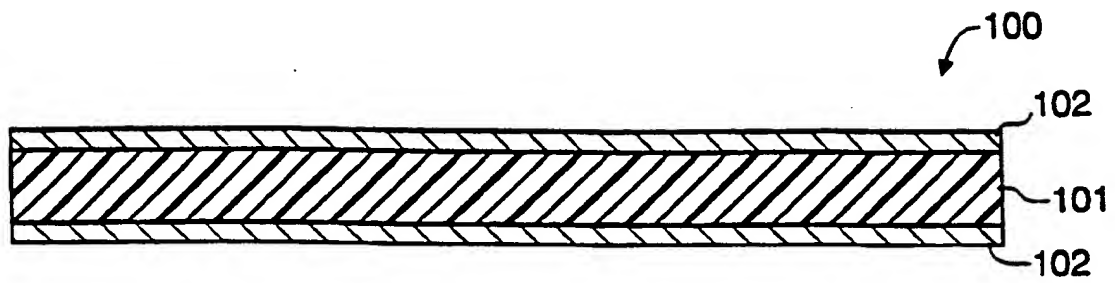| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2770 | OH2 | TIP3 | 91 | 98.629 | 61.636 | 27.795 | 1.00 | 44.47 |
| ATOM | 2771 | OH2 | TIP3 | 93 | 92.075 | 77.451 | 42.668 | 1.00 | 46.15 |
| ATOM | 2772 | OH2 | TIP3 | 94 | 94.761 | 55.023 | 38.581 | 1.00 | 43.31 |
| ATOM | 2773 | OH2 | TIP3 | 95 | 94.860 | 63.387 | 30.662 | 1.00 | 23.26 |
| ATOM | 2774 | OH2 | TIP3 | 97 | 96.495 | 61.394 | 31.222 | 1.00 | 17.95 |
| ATOM | 2775 | OH2 | TIP3 | 99 | 97.135 | 61.058 | 33.735 | 1.00 | 24.21 |
| ATOM | 2776 | OH2 | TIP3 | 100 | 98.598 | 62.340 | 24.703 | 1.00 | 15.55 |
| ATOM | 2777 | OH2 | TIP3 | 101 | 96.091 | 63.609 | 25.209 | 1.00 | 16.64 |
| ATOM | 2778 | OH2 | TIP3 | 102 | 95.591 | 62.210 | 28.267 | 1.00 | 28.35 |
| ATOM | 2779 | OH2 | TIP3 | 103 | 84.181 | 68.384 | 51.386 | 1.00 | 37.36 |
| ATOM | 2780 | OH2 | TIP3 | 104 | 90.542 | 76.184 | 46.889 | 1.00 | 50.54 |
| ATOM | 2781 | OH2 | TIP3 | 105 | 87.338 | 52.422 | 55.348 | 1.00 | 57.64 |
| ATOM | 2782 | OH2 | TIP3 | 106 | 86.485 | 55.114 | 55.782 | 1.00 | 53.13 |
| ATOM | 2783 | OH2 | TIP3 | 107 | 71.978 | 33.253 | 38.083 | 1.00 | 37.67 |
| ATOM | 2784 | OH2 | TIP3 | 108 | 86.389 | 52.030 | 52.810 | 1.00 | 45.08 |
| ATOM | 2785 | OH2 | TIP3 | 109 | 88.375 | 44.898 | 51.380 | 1.00 | 45.72 |
| ATOM | 2786 | OH2 | TIP3 | 110 | 76.040 | 31.693 | 38.282 | 1.00 | 49.11 |
| ATOM | 2787 | OH2 | TIP3 | 111 | 88.171 | 23.460 | 70.887 | 1.00 | 34.87 |
| ATOM | 2788 | OH2 | TIP3 | 112 | 81.925 | 26.203 | 48.120 | 1.00 | 34.21 |
| ATOM | 2789 | OH2 | TIP3 | 113 | 75.036 | 35.002 | 37.397 | 1.00 | 43.93 |
| ATOM | 2790 | OH2 | TIP3 | 114 | 66.842 | 37.170 | 41.543 | 1.00 | 37.92 |
| ATOM | 2791 | OH2 | TIP3 | 115 | 74.137 | 22.561 | 64.810 | 1.00 | 39.94 |
| ATOM | 2792 | OH2 | TIP3 | 116 | 75.230 | 29.105 | 47.361 | 1.00 | 33.31 |
| ATOM | 2793 | OH2 | TIP3 | 117 | 71.548 | 35.570 | 75.085 | 1.00 | 51.53 |
| ATOM | 2794 | OH2 | TIP3 | 118 | 91.190 | 40.939 | 65.032 | 1.00 | 59.85 |
| ATOM | 2795 | OH2 | TIP3 | 119 | 89.208 | 54.691 | 55.131 | 1.00 | 49.67 |
| ATOM | 2796 | OH2 | TIP3 | 120 | 87.603 | 20.791 | 70.317 | 1.00 | 41.15 |
| ATOM | 2797 | OH2 | TIP3 | 121 | 82.007 | 24.661 | 44.978 | 1.00 | 44.91 |
| ATOM | 2798 | OH2 | TIP3 | 122 | 67.254 | 62.385 | 54.134 | 1.00 | 55.45 |
| ATOM | 2799 | OH2 | TIP3 | 123 | 69.652 | 50.335 | 60.131 | 1.00 | 56.04 |
| ATOM | 2800 | OH2 | TIP3 | 124 | 91.100 | 35.309 | 64.126 | 1.00 | 10.24 |
| ATOM | 2801 | OH2 | TIP3 | 125 | 75.803 | 55.613 | 55.160 | 1.00 | 19.38 |
| ATOM | 2802 | OH2 | TIP3 | 126 | 67.414 | 58.406 | 48.372 | 1.00 | 50.59 |
| ATOM | 2803 | OH2 | TIP3 | 127 | 61.992 | 60.345 | 41.276 | 1.00 | 54.28 |
| ATOM | 2804 | OH2 | TIP3 | 128 | 100.397 | 72.990 | 35.528 | 1.00 | 47.93 |
| ATOM | 2805 | OH2 | TIP3 | 129 | 78.374 | 54.246 | 34.009 | 1.00 | 25.64 |
| ATOM | 2806 | OH2 | TIP3 | 130 | 74.448 | 74.269 | 39.281 | 1.00 | 43.21 |
| ATOM | 2807 | OH2 | TIP3 | 131 | 64.202 | 44.752 | 43.474 | 1.00 | 49.87 |
| ATOM | 2808 | OH2 | TIP3 | 132 | 88.521 | 75.111 | 27.052 | 1.00 | 58.72 |
| ATOM | 2809 | OH2 | TIP3 | 133 | 69.530 | 56.754 | 48.247 | 1.00 | 28.48 |
| ATOM | 2810 | OH2 | TIP3 | 134 | 79.780 | 77.649 | 41.569 | 1.00 | 58.74 |
| ATOM | 2811 | OH2 | TIP3 | 135 | 88.780 | 33.735 | 64.655 | 1.00 | 36.24 |
| ATOM | 2812 | OH2 | TIP3 | 136 | 104.389 | 57.542 | 20.144 | 1.00 | 59.52 |
| ATOM | 2813 | OH2 | TIP3 | 137 | 64.410 | 59.785 | 53.812 | 1.00 | 52.08 |
| ATOM | 2814 | OH2 | TIP3 | 138 | 99.184 | 58.625 | 27.266 | 1.00 | 30.88 |
| ATOM | 2815 | OH2 | TIP3 | 139 | 101.746 | 57.264 | 20.715 | 1.00 | 37.99 |

END
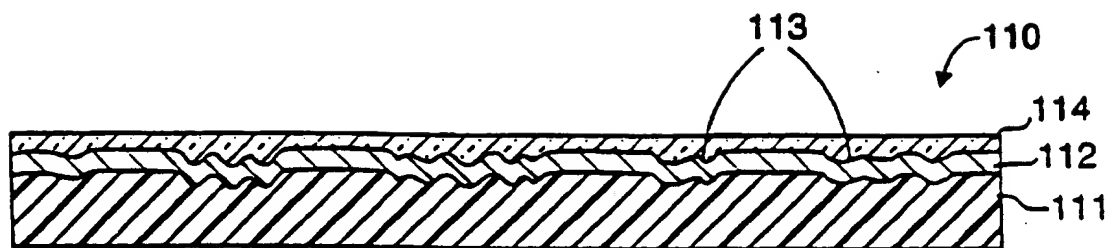
60/60



Figure 5



Figure 6

| A. CLASSIFICATION OF SUBJECT MATTER |
|---|
| IPC 6    C07K14/18    C07K1/00    G06F17/50    C30B7/00 |

According to International Patent Classification(IPC) or to both national classification and IPC

| B. FIELDS SEARCHED |
|---|
| Minimum documentation searched (classification system followed by classification symbols) |
| IPC 6    C07K   G06F   C30B |

Documentation searched other than minimumdocumentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and. where practical. search terms used)

### C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category * | Citation of document. with indication. where appropriate. of the relevant passages | Relevant to claim No. |
|---|---|---|
| X | C LIN ET AL.: "A central region in the hepatitis C virus NS4A protein allows formation of an active NS3-NS4A serine proteinase complex in vivo and in vitro" JOURNAL OF VIROLOGY., vol. 69, no. 7, July 1995, AMERICAN SOCIETY FOR MICROBIOLOGY    US, pages 4373-4380, XP002053691 see the whole document<br><br>---<br><br>-/-- | 1-3 |

[X] Further documents are listed in the continuation of box C.      [X] Patent family members are listed in annex.

* Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or . which is cited to establish the publicationdate of another citation or other special reason (as specified)

"O" document referring to an oral disclosure. use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

| Date of the actual completion of theinternational search | Date of mailing of the international search report |
|---|---|
| 28 January 1998 | 13/02/1998 |

| Name and mailing address of the ISA | Authorized officer |
|---|---|
| European Patent Office. P.B. 5818 Patentlaan 2<br>NL - 2280 HV Rijswijk<br>Tel. (+31-70) 340-2040. Tx. 31 651 epo nl.<br>Fax: (+31-70) 340-3016 | Masturzo, P |

Form PCT/ISA/210 (second sheet) (July 1992)

PCT/US 97/16182

| Category | Citation of document. with indication,where appropriate, of the relevant passages | Relevant to claim No. |
|---|---|---|
| X | R BARTENSCHLAGER ET AL.: "Complex formation between the NS3 serine-type proteinase of the hepatitis C virus and NS4A and its importance for polyprotein maturation " JOURNAL OF VIROLOGY., vol. 69, no. 12, December 1995, AMERICAN SOCIETY FOR MICROBIOLOGY US, pages 7519-7528, XP002053692 see the whole document --- | 1,2 |
| X | WO 95 22985 A (ISTITUTO ANGELETTI) 31 August 1995 see claims 5,6 --- | 1,2 |
| P,X | J L KIM ET AL.: "Crystal structure of the hepatitis C virus NS3 protease domain complexed with a synthetic NS4A cofactor peptide" CELL, vol. 87, 18 October 1996, NA US, pages 343-355, XP002053693 see the whole document ----- | 1-14 |

**C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT**

| Patent document cited in search report | Publication date | Patent family member(s) | Publication date |
|---|---|---|---|
| WO 9522985 A | 31-08-95 | IT 1272179 B | 16-06-97 |
| | | AU 1822395 A | 11-09-95 |
| | | CA 2182521 A | 31-08-95 |
| | | EP 0746333 A | 11-12-96 |